Connecting via Winsock to STN

Welcome to STN International!  Enter x:x

LOGINID:ssptajsl1623

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

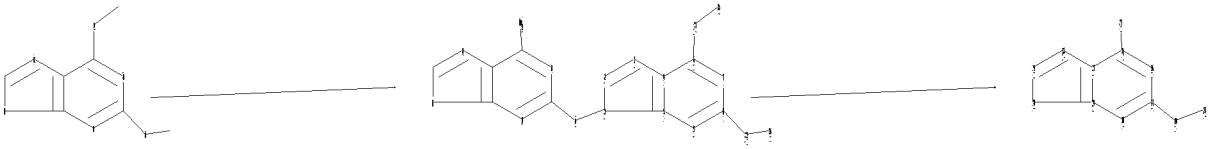
* * * * * * * * * *  Welcome to STN International  * * * * * * * * * *

| | | |
|---|---|---|
| NEWS 1 | | Web Page for STN Seminar Schedule - N. America |
| NEWS 2 | APR 02 | CAS Registry Number Crossover Limits Increased to 500,000 in Key STN Databases |
| NEWS 3 | APR 02 | PATDPAFULL: Application and priority number formats enhanced |
| NEWS 4 | APR 02 | DWPI: New display format ALLSTR available |
| NEWS 5 | APR 02 | New Thesaurus Added to Derwent Databases for Smooth Sailing through U.S. Patent Codes |
| NEWS 6 | APR 02 | EMBASE Adds Unique Records from MEDLINE, Expanding Coverage back to 1948 |
| NEWS 7 | APR 07 | 50,000 World Traditional Medicine (WTM) Patents Now Available in CAplus |
| NEWS 8 | APR 07 | MEDLINE Coverage Is Extended Back to 1947 |
| NEWS 9 | JUN 16 | WPI First View (File WPIFV) will no longer be available after July 30, 2010 |
| NEWS 10 | JUN 18 | DWPI: New coverage - French Granted Patents |
| NEWS 11 | JUN 18 | CAS and FIZ Karlsruhe announce plans for a new STN platform |
| NEWS 12 | JUN 18 | IPC codes have been added to the INSPEC backfile (1969-2009) |
| NEWS 13 | JUN 21 | Removal of Pre-IPC 8 data fields streamline displays in CA/CAplus, CASREACT,and MARPAT |
| NEWS 14 | JUN 21 | Access an additional 1.8 million records exclusively enhanced with 1.9 million CAS Registry Numbers -- EMBASE Classic on STN |
| NEWS 15 | JUN 28 | Introducing "CAS Chemistry Research Report": 40 Years of Biofuel Research Reveal China Now Atop U.S. in Patenting and Commercialization of Bioethanol |
| NEWS 16 | JUN 29 | Enhanced Batch Search Options in DGENE, USGENE, and PCTGEN |
| NEWS 17 | JUL 19 | Enhancement of citation information in INPADOC databases provides new, more efficient competitor analyses |
| NEWS 18 | JUL 26 | CAS coverage of global patent authorities has expanded to 61 with the addition of Costa Rica |
| NEWS 19 | SEP 15 | MEDLINE Cited References provide additional revelant records with no additional searching. |
| NEWS 20 | OCT 04 | Removal of Pre-IPC 8 data fields streamlines displays in USPATFULL, USPAT2, and USPATOLD. |
| NEWS 21 | OCT 04 | Precision of EMBASE searching enhanced with new chemical name field |
| NEWS 22 | OCT 06 | Increase your retrieval consistency with new formats or for Taiwanese application numbers in CA/CAplus. |

```
 NEWS 23  OCT 21  CA/CAplus kind code changes for Chinese patents
                  increase consistency, save time
 NEWS 24  OCT 22  New version of STN Viewer preserves custom
                  highlighting of terms when patent documents are
                  saved in .rtf format
 NEWS 25  OCT 28  INPADOCDB/INPAFAMDB: Enhancements to the US national
                  patent classification.
 NEWS 26  NOV 03  New format for Korean patent application numbers in
                  CA/CAplus increases consistency, saves time.
 NEWS 27  NOV 04  Selected STN databases scheduled for removal on
                  December 31, 2010

 NEWS EXPRESS FEBRUARY 15 10 CURRENT WINDOWS VERSION IS V8.4.2,
          AND CURRENT DISCOVER FILE IS DATED 07 JULY 2010.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that
specific topic.

  All use of STN is subject to the provisions of the STN customer
  agreement.  This agreement limits use to scientific research.  Use
  for software development or design, implementation of commercial
  gateways, or use of CAS and STN data in the building of commercial
  products is prohibited and may result in loss of user privileges
  and other penalties.

* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 15:07:09 ON 10 NOV 2010

=> b reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.22       0.22

FILE 'REGISTRY' ENTERED AT 15:07:25 ON 10 NOV 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2010 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:    9 NOV 2010  HIGHEST RN 1252174-83-6
DICTIONARY FILE UPDATES:   9 NOV 2010  HIGHEST RN 1252174-83-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:
```

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\jlau1\My Documents\10581544 - spongosine\rxn search.str



chain nodes :
21 22 23 24 25 26 27
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
chain bonds :
6-21 8-22 15-23 17-24 21-25 22-26 24-27
ring bonds :
1-2 1-5 2-3 3-4 4-5 4-6 5-9 6-7 7-8 8-9 10-11 10-14 11-12 12-13 13-14 13-15 14-18 15-16 16-17 17-18
exact/norm bonds :
1-2 1-5 2-3 3-4 6-21 8-22 10-11 10-14 11-12 12-13 15-23 17-24 21-25 22-26 24-27
normalized bonds :
4-5 4-6 5-9 6-7 7-8 8-9 13-14 13-15 14-18 15-16 16-17 17-18

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS
fragments assigned product role:
containing 10
fragments assigned reactant/reagent role:
containing 1

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> b stng
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION

FULL ESTIMATED COST 0.49 0.71

FILE 'STNGUIDE' ENTERED AT 15:07:59 ON 10 NOV 2010
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Nov 5, 2010 (20101105/UP).

=> b casreact

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 0.07 | 0.78 |

FILE 'CASREACT' ENTERED AT 15:08:06 ON 10 NOV 2010
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)



FILE CONTENT:1840 - 7 Nov 2010 VOL 153 ISS 20

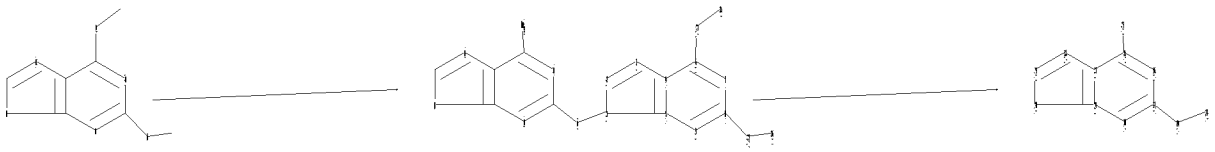
New CAS Information Use Policies, enter HELP USAGETERMS for details.

CASREACT now has more than 22.7 million single and multi-step
reactions.

CASREACT contains reactions from CAS and from: ZIC/VINITI database
(1974-1999) provided by InfoChem; INPI data prior to 1986;
Biotransformations database compiled under the direction of
Professor Dr. Klaus Kieslich; organic reactions, portions copyright
1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc.,
Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under
license. All Rights Reserved.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=>
Uploading C:\Documents and Settings\jlau1\My Documents\10581544 - spongosine\rxn
search.str



chain nodes :
21 22 23 24 25 26 27
ring nodes :

```
1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17  18
chain bonds :
6-21  8-22  15-23  17-24  21-25  22-26  24-27
ring bonds :
1-2  1-5  2-3  3-4  4-5  4-6  5-9  6-7  7-8  8-9  10-11  10-14  11-12  12-13  13-14
 13-15  14-18  15-16  16-17  17-18
exact/norm bonds :
1-2  1-5  2-3  3-4  6-21  8-22  10-11  10-14  11-12  12-13  15-23  17-24  21-25
22-26  24-27
normalized bonds :
4-5  4-6  5-9  6-7  7-8  8-9  13-14  13-15  14-18  15-16  16-17  17-18


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  21:CLASS
22:CLASS  23:CLASS  24:CLASS  25:CLASS  26:CLASS  27:CLASS
fragments assigned product role:
containing 10
fragments assigned reactant/reagent role:
containing 1




L2      STRUCTURE UPLOADED

=> d l2
L2 HAS NO ANSWERS
L2              STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


<------User Break------>

=> b stng
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.49       1.27

FILE 'STNGUIDE' ENTERED AT 15:08:35 ON 10 NOV 2010
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Nov  5, 2010 (20101105/UP).

=> logoff hold
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.84       2.11

 SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 15:15:55 ON 10 NOV 2010

Connecting via Winsock to STN
```

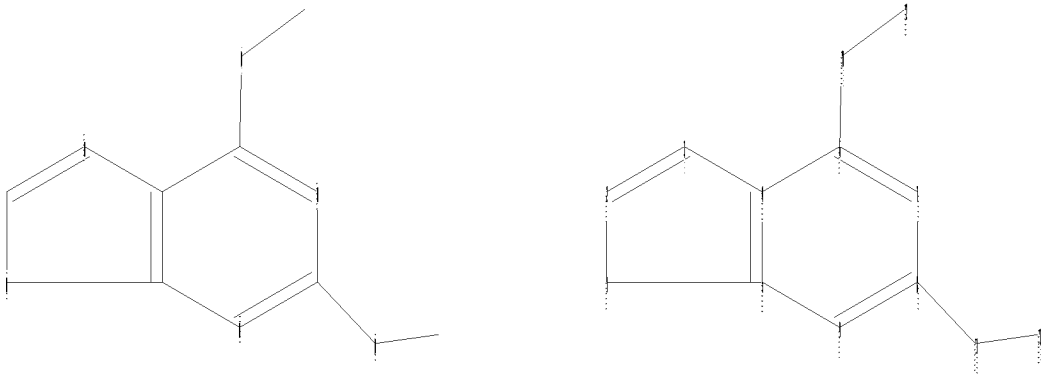
```
Welcome to STN International!  Enter x:
x
Welcome to STN International!  Enter x:
LOGINID:ssptajsl1623

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2


* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1           Web Page for STN Seminar Schedule - N. America
 NEWS  2  APR 02   CAS Registry Number Crossover Limits Increased to
                   500,000 in Key STN Databases
 NEWS  3  APR 02   PATDPAFULL: Application and priority number formats
                   enhanced
 NEWS  4  APR 02   DWPI: New display format ALLSTR available
 NEWS  5  APR 02   New Thesaurus Added to Derwent Databases for Smooth
                   Sailing through U.S. Patent Codes
 NEWS  6  APR 02   EMBASE Adds Unique Records from MEDLINE, Expanding
                   Coverage back to 1948
 NEWS  7  APR 07   50,000 World Traditional Medicine (WTM) Patents Now
                   Available in CAplus
 NEWS  8  APR 07   MEDLINE Coverage Is Extended Back to 1947
 NEWS  9  JUN 16   WPI First View (File WPIFV) will no longer be
                   available after July 30, 2010
 NEWS 10  JUN 18   DWPI: New coverage - French Granted Patents
 NEWS 11  JUN 18   CAS and FIZ Karlsruhe announce plans for a new
                   STN platform
 NEWS 12  JUN 18   IPC codes have been added to the INSPEC backfile
                   (1969-2009)
 NEWS 13  JUN 21   Removal of Pre-IPC 8 data fields streamline displays
                   in CA/CAplus, CASREACT,and MARPAT
 NEWS 14  JUN 21   Access an additional 1.8 million records exclusively
                   enhanced with 1.9 million CAS Registry Numbers --
                   EMBASE Classic on STN
 NEWS 15  JUN 28   Introducing "CAS Chemistry Research Report": 40 Years
                   of Biofuel Research Reveal China Now Atop U.S. in
                   Patenting and Commercialization of Bioethanol
 NEWS 16  JUN 29   Enhanced Batch Search Options in DGENE, USGENE,
                   and PCTGEN
 NEWS 17  JUL 19   Enhancement of citation information in INPADOC
                   databases provides new, more efficient competitor
                   analyses
 NEWS 18  JUL 26   CAS coverage of global patent authorities has
                   expanded to 61 with the addition of Costa Rica
 NEWS 19  SEP 15   MEDLINE Cited References provide additional
                   revelant records with no additional searching.
 NEWS 20  OCT 04   Removal of Pre-IPC 8 data fields streamlines
                   displays in USPATFULL, USPAT2, and USPATOLD.
 NEWS 21  OCT 04   Precision of EMBASE searching enhanced with new
                   chemical name field
 NEWS 22  OCT 06   Increase your retrieval consistency with new formats  or
                   for Taiwanese application numbers in CA/CAplus.
 NEWS 23  OCT 21   CA/CAplus kind code changes for Chinese patents
```

```
                  increase consistency, save time
 NEWS 24  OCT 22  New version of STN Viewer preserves custom
                  highlighting of terms when patent documents are
                  saved in .rtf format
 NEWS 25  OCT 28  INPADOCDB/INPAFAMDB: Enhancements to the US national
                  patent classification.
 NEWS 26  NOV 03  New format for Korean patent application numbers in
                  CA/CAplus increases consistency, saves time.
 NEWS 27  NOV 04  Selected STN databases scheduled for removal on
                  December 31, 2010

 NEWS EXPRESS FEBRUARY 15 10 CURRENT WINDOWS VERSION IS V8.4.2,
          AND CURRENT DISCOVER FILE IS DATED 07 JULY 2010.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that
specific topic.

  All use of STN is subject to the provisions of the STN customer
  agreement.  This agreement limits use to scientific research.  Use
  for software development or design, implementation of commercial
  gateways, or use of CAS and STN data in the building of commercial
  products is prohibited and may result in loss of user privileges
  and other penalties.

* * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 08:38:27 ON 12 NOV 2010

=> b reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.22       0.22

FILE 'REGISTRY' ENTERED AT 08:38:42 ON 12 NOV 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2010 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   11 NOV 2010  HIGHEST RN 1252761-16-2
DICTIONARY FILE UPDATES:  11 NOV 2010  HIGHEST RN 1252761-16-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:
```

http://www.cas.org/support/stngen/stndoc/properties.html

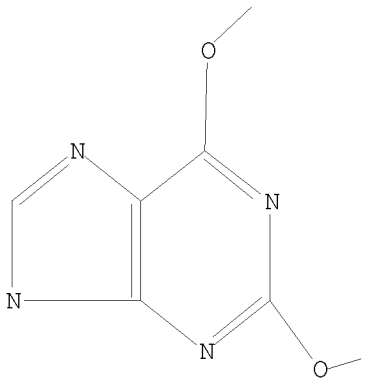
```
=> e adenosine, 4,6-dimethoxy/cn
E1            1     ADENOSINE, 4,5-DIDEHYDRO-2,5-DIDEOXY-, 3'-ACETATE/CN
E2            1     ADENOSINE, 4,5-DIHYDRO-5-(2-OXOBUTYL)-/CN
E3            0 --> ADENOSINE, 4,6-DIMETHOXY/CN
E4            2     ADENOSINE, 4-(1-AZIRIDINYL)-4-DEAMINO-2'-DEOXYCYTIDYLYL-(3'.
                    FWDARW.5')-2'-DEOXY-5-METHYLCYTIDYLYL-(3'.FWDARW.5')-THYMIDY
                    LYL-(3'.FWDARW.5')-THYMIDYLYL-(3'.FWDARW.5')-THYMIDYLYL-(3'.
                    FWDARW.5')-THYMIDYLY/CN
E5            2     ADENOSINE, 4-(1-AZIRIDINYL)-4-DEAMINO-2'-DEOXYCYTIDYLYL-(3'.
                    FWDARW.5')-2'-DEOXY-7,8-DIHYDRO-N-METHYL-8-OXOADENYLYL-(3'.F
                    WDARW.5')-2'-DEOXY-5-METHYLCYTIDYLYL-(3'.FWDARW.5')-THYMIDYL
                    YL-(3'.FWDARW.5')-TH/CN
E6            5     ADENOSINE, 4-(1-AZIRIDINYL)-4-DEAMINO-2'-DEOXYCYTIDYLYL-(3'.
                    FWDARW.5')-2'-DEOXY-7,8-DIHYDRO-N-METHYL-8-OXOADENYLYL-(3'.F
                    WDARW.5')-2'-DEOXY-7,8-DIHYDRO-N-METHYL-8-OXOADENYLYL-(3'.FW
                    DARW.5')-2'-DEOXY-7,/CN
E7            3     ADENOSINE, 4-(1-AZIRIDINYL)-4-DEAMINO-2'-DEOXYCYTIDYLYL-(3'.
                    FWDARW.5')-2'-DEOXY-7,8-DIHYDRO-N-METHYL-8-OXOADENYLYL-(3'.F
                    WDARW.5')-2'-DEOXY-7,8-DIHYDRO-N-METHYL-8-OXOADENYLYL-(3'.FW
                    DARW.5')-THYMIDYLYL-/CN
E8            3     ADENOSINE, 4-(1-AZIRIDINYL)-4-DEAMINO-2'-DEOXYCYTIDYLYL-(3'.
                    FWDARW.5')-2'-DEOXY-7,8-DIHYDRO-N-METHYL-8-OXOADENYLYL-(3'.F
                    WDARW.5')-THYMIDYLYL-(3'.FWDARW.5')-THYMIDYLYL-(3'.FWDARW.5'
                    )-THYMIDYLYL-(3'.FWD/CN
E9            4     ADENOSINE, 4-(1-AZIRIDINYL)-4-DEAMINO-2'-DEOXYCYTIDYLYL-(3'.
                    FWDARW.5')-THYMIDYLYL-(3'.FWDARW.5')-2'-DEOXY-7,8-DIHYDRO-N-
                    METHYL-8-OXOADENYLYL-(3'.FWDARW.5')-2'-DEOXY-7,8-DIHYDRO-N-M
                    ETHYL-8-OXOADENYLYL-/CN
E10           1     ADENOSINE, 4-(1-AZIRIDINYL)-4-DEAMINO-2'-DEOXYCYTIDYLYL-(3'.
                    FWDARW.5')-THYMIDYLYL-(3'.FWDARW.5')-2'-DEOXY-7,8-DIHYDRO-N-
                    METHYL-8-OXOADENYLYL-(3'.FWDARW.5')-THYMIDYLYL-(3'.FWDARW.5'
                    )-THYMIDYLYL-(3'.FWD/CN
E11           2     ADENOSINE, 4-(1-AZIRIDINYL)-4-DEAMINO-2'-DEOXYCYTIDYLYL-(3'.
                    FWDARW.5')-THYMIDYLYL-(3'.FWDARW.5')-THYMIDYLYL-(3'.FWDARW.5
                    ')-2'-DEOXY-5-METHYLCYTIDYLYL-(3'.FWDARW.5')-THYMIDYLYL-(3'.
                    FWDARW.5')-THYMIDYLY/CN
E12           1     ADENOSINE, 4-(1-AZIRIDINYL)-4-DEAMINO-2'-DEOXYCYTIDYLYL-(3'.
                    FWDARW.5')-THYMIDYLYL-(3'.FWDARW.5')-THYMIDYLYL-(3'.FWDARW.5
                    ')-2'-DEOXY-7,8-DIHYDRO-N-METHYL-8-OXOADENYLYL-(3'.FWDARW.5'
                    )-2'-DEOXY-7,8-DIHYD/CN

=> e purine, 4,6-dimethoxy/cn
E1            1     PURINE, 3,6-DIHYDRO-6-IMINO-3-METHYL-/CN
E2            1     PURINE, 3-OXIDE/CN
E3            0 --> PURINE, 4,6-DIMETHOXY/CN
E4            1     PURINE, 6,6'-((5-NITRO-4,6-PYRIMIDINEDIYL)DITHIO)DI-/CN
E5            1     PURINE, 6,6'-((6-CHLORO-2,4-PYRIMIDINEDIYL)DITHIO)BIS(2-AMIN
                    O-/CN
E6            1     PURINE, 6,6'-(1,3,4-THIADIAZOLE-2,5-DIYLDITHIO)DI-/CN
E7            1     PURINE, 6,6'-(1,4-PIPERAZINEDIYL)DI-/CN
E8            1     PURINE, 6,6'-(1,4-PIPERAZINEDIYL)DI-, DIPICRATE/CN
E9            1     PURINE, 6,6'-(ETHYLENEDITHIO)DI-/CN
E10           1     PURINE, 6,6'-(HEXAMETHYLENEDITHIO)DI-/CN
E11           1     PURINE, 6,6'-(IMINOETHYLENE)DI-/CN
E12           1     PURINE, 6,6'-(IMINOTRIMETHYLENE)DI-/CN

=> b stng
```

```
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.98       1.20

FILE 'STNGUIDE' ENTERED AT 08:39:46 ON 12 NOV 2010
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Nov  5, 2010 (20101105/UP).

=> b reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.28       1.48

FILE 'REGISTRY' ENTERED AT 08:42:20 ON 12 NOV 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2010 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   11 NOV 2010  HIGHEST RN 1252761-16-2
DICTIONARY FILE UPDATES:  11 NOV 2010  HIGHEST RN 1252761-16-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\jlau1\My Documents\10581544 -
spongosine\reagent.str
```



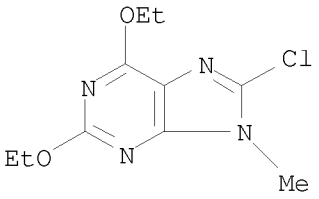
```
chain nodes :
10  11  12  13
```

```
ring nodes :
1  2  3  4  5  6  7  8  9
chain bonds :
6-10  8-11  10-12  11-13
ring bonds :
1-2  1-5  2-3  3-4  4-5  4-6  5-9  6-7  7-8  8-9
exact/norm bonds :
1-2  1-5  2-3  3-4  6-10  8-11  10-12  11-13
normalized bonds :
4-5  4-6  5-9  6-7  7-8  8-9


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:CLASS
11:CLASS  12:CLASS  13:CLASS



L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR
```




```
Structure attributes must be viewed using STN Express query preparation.


=> s l1 sss sam
SAMPLE SEARCH INITIATED 08:42:34 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      252 TO ITERATE

100.0% PROCESSED      252 ITERATIONS                                5 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          4088 TO     5992
PROJECTED ANSWERS:                5 TO      234

L2            5 SEA SSS SAM L1

=> d l2 scan
```

L2  5 ANSWERS  REGISTRY  COPYRIGHT 2010 ACS on STN
IN  9H-Purine, 8-chloro-2,6-diethoxy-9-methyl-
MF  C10 H13 Cl N4 O2

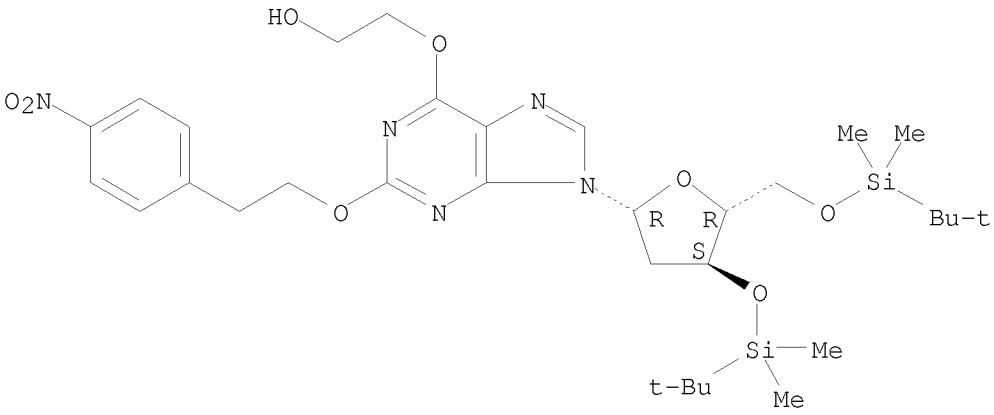



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2  5 ANSWERS  REGISTRY  COPYRIGHT 2010 ACS on STN
IN  Xanthosine, 2'-deoxy-3',5'-bis-O-[(1,1-dimethylethyl)dimethylsilyl]-6-O-(2-hydroxyethyl)-2-O-[2-(4-nitrophenyl)ethyl]- (9CI)
MF  C32 H51 N5 O8 Si2

Absolute stereochemistry.

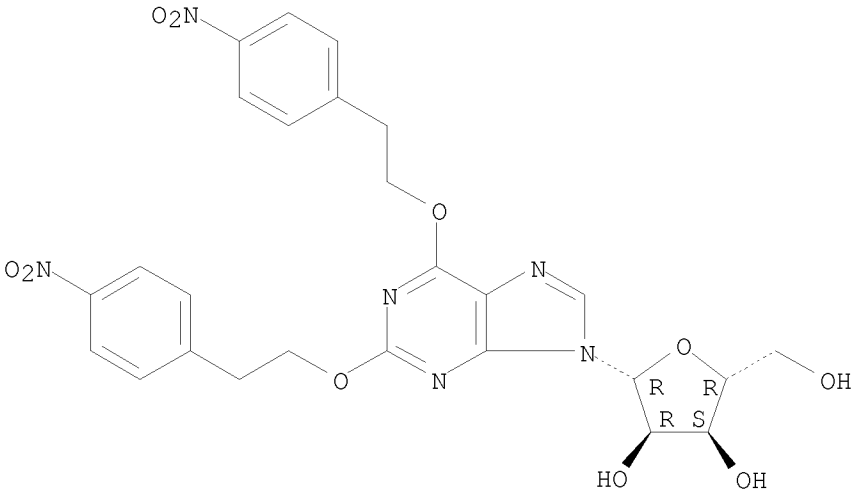



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2  5 ANSWERS  REGISTRY  COPYRIGHT 2010 ACS on STN
IN  Xanthosine, 2,6-bis-O-[2-(4-nitrophenyl)ethyl]- (9CI)
MF  C26 H26 N6 O10

Absolute stereochemistry.

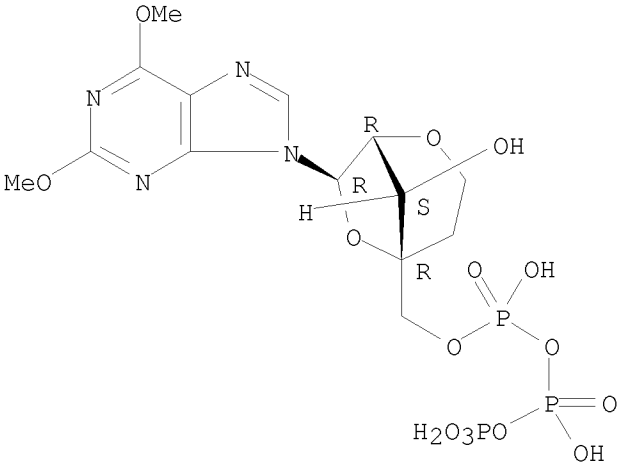


**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 5 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 9H-Purine, 9-[2,6-anhydro-5-deoxy-4-C-(3,5,7,7-tetrahydroxy-3,5,7-trioxido-2,4,6-trioxa-3,5,7-triphosphahept-1-yl)-α-L-lyxo-hexofuranosyl]-2,6-dimethoxy- (9CI)
MF C14 H21 N4 O15 P3

Absolute stereochemistry.



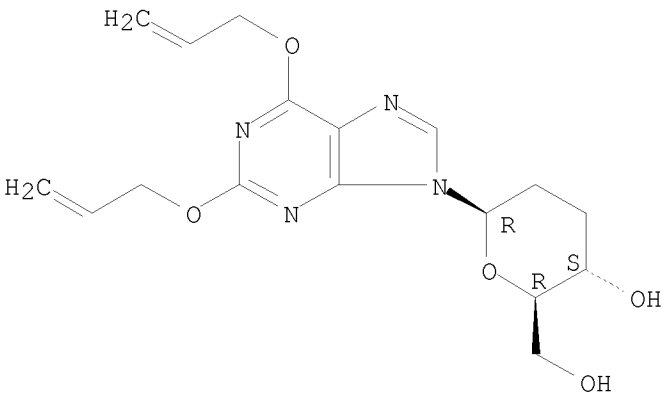
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 5 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN 9H-Purine, 9-(2,3-dideoxy-β-D-erythro-hexopyranosyl)-2,6-bis(2-propenyloxy)- (9CI)

MF  C17 H22 N4 O5

Absolute stereochemistry.  Rotation (-).

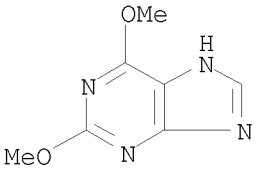


**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

ALL ANSWERS HAVE BEEN SCANNED

```
=> e 9H-purine, 2,6-dimethoxy/cn
E1            1     9H-PURINE, 2,6-DIIODO-/CN
E2            1     9H-PURINE, 2,6-DIIODO-9-(2,3,5-TRI-O-ACETYL-B-D-RIBOFUR
                    ANOSYL)-/CN
E3            0 --> 9H-PURINE, 2,6-DIMETHOXY/CN
E4            1     9H-PURINE, 2,6-DIMETHOXY-/CN
E5            1     9H-PURINE, 2,6-DIMETHYL-/CN
E6            1     9H-PURINE, 2,6-DIMETHYL-8-PROPYL-9-((2'-(1H-TETRAZOL-5-YL)(1
                    ,1'-BIPHENYL)-4-YL)METHYL)-/CN
E7            1     9H-PURINE, 2,6-DIMETHYL-8-PROPYL-9-((2'-(2H-TETRAZOL-5-YL)(1
                    ,1'-BIPHENYL)-4-YL)METHYL)-/CN
E8            1     9H-PURINE, 2,6-DIMETHYL-9-(2,3,5-TRI-O-BENZOYL-B-D-RIBO
                    FURANOSYL)-/CN
E9            1     9H-PURINE, 2,6-DIMETHYL-9-(4-(1-METHYLETHYL)-2-(METHYLTHIO)P
                    HENYL)-/CN
E10           1     9H-PURINE, 2,6-DIMETHYL-9-(PHENYLMETHYL)-/CN
E11           1     9H-PURINE, 2,6-DIMETHYL-9-(TETRAHYDRO-2H-PYRAN-2-YL)-/CN
E12           1     9H-PURINE, 2,6-DIMETHYL-9-B-D-RIBOFURANOSYL-/CN

=> s e4
L3            1 "9H-PURINE, 2,6-DIMETHOXY-"/CN

=> d l3

L3   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2010 ACS on STN
RN   5327-19-5  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   9H-Purine, 2,6-dimethoxy-  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   1H-Purine, 2,6-dimethoxy- (9CI)
OTHER NAMES:
CN   NSC 3295
MF   C7 H8 N4 O2
```

LC  STN Files:  BEILSTEIN*, CA, CAPLUS, CHEMCATS
        (*File contains numerically searchable property data)




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> e adenosine, 2,6-dimethoxy-/cn
E1  1  ADENOSINE, 2,5'-DICHLORO-N-CYCLOPENTYL-5'-DEOXY-2'-C-METHYL-/CN
E2  1  ADENOSINE, 2,5'-DICHLORO-N-CYCLOPENTYL-5'-DEOXY-2'-C-METHYL-2',3'-O-(1-METHYLETHYLIDENE)-/CN
E3  0 --> ADENOSINE, 2,6-DIMETHOXY-/CN
E4  1  ADENOSINE, 2,8-BIS((4-CHLOROPHENYL)THIO)-, CYCLIC 3',5'-(HYDROGEN PHOSPHATE)/CN
E5  1  ADENOSINE, 2,8-BIS((PHENYLMETHYL)AMINO)-/CN
E6  1  ADENOSINE, 2,8-BIS(1-HYDROXY-1-METHYLETHYL)-/CN
E7  1  ADENOSINE, 2,8-BIS(AMINOCARBONYL)-N-BENZOYL-, 2',3',5'-TRIACETATE/CN
E8  1  ADENOSINE, 2,8-BIS(BUTYLTHIO)-, CYCLIC 3',5'-(HYDROGEN PHOSPHATE)/CN
E9  1  ADENOSINE, 2,8-BIS(METHYLTHIO)-/CN
E10  1  ADENOSINE, 2,8-BIS(METHYLTHIO)-, TRIACETATE/CN
E11  1  ADENOSINE, 2,8-BIS(METHYLTHIO)-, TRIBENZOATE/CN
E12  1  ADENOSINE, 2,8-DI-1-HEXYNYL-/CN

=> e
E13  1  ADENOSINE, 2,8-DIACETYL-N-BENZOYL-, 2',3',5'-TRIACETATE/CN
E14  1  ADENOSINE, 2,8-DIAMINO-/CN
E15  1  ADENOSINE, 2,8-DIAMINO-, CYCLIC 3',5'-(HYDROGEN PHOSPHATE)/CN
E16  1  ADENOSINE, 2,8-DIAMINO-2',3'-DIDEOXY-/CN
E17  1  ADENOSINE, 2,8-DIAZIDO-/CN
E18  1  ADENOSINE, 2,8-DIBROMO-, CYCLIC 3',5'-(HYDROGEN PHOSPHATE)/CN
E19  1  ADENOSINE, 2,8-DICHLORO-/CN
E20  1  ADENOSINE, 2,8-DICHLORO-2',3'-O-ISOPROPYLIDENE-/CN
E21  1  ADENOSINE, 2,8-DICHLORO-2',3'-O-ISOPROPYLIDENE-, 5'-P-TOLUENESULFONATE/CN
E22  1  ADENOSINE, 2,8-DICHLORO-2'-DEOXY-/CN
E23  1  ADENOSINE, 2,8-DICHLORO-2'-DEOXY-, DIACETATE/CN
E24  1  ADENOSINE, 2,8-DICHLORO-5'-DEOXY-5'-IODO-/CN

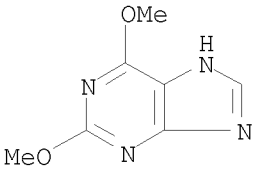
=> e
E25  1  ADENOSINE, 2,8-DICHLORO-5'-DEOXY-5'-IODO-, 2',3'-DIACETATE/CN
E26  1  ADENOSINE, 2,8-DICHLORO-5'-DEOXY-5'-IODO-2',3'-O-ISOPROPYLID

```
                  ENE-/CN
E27          1    ADENOSINE, 2,8-DICHLORO-5'-S-METHYL-5'-THIO-/CN
E28          1    ADENOSINE, 2,8-DICHLORO-5'-S-METHYL-5'-THIO-, 2',3'-DIACETAT
                  E/CN
E29          1    ADENOSINE, 2,8-DICHLORO-5'-S-METHYL-5'-THIO-, DIACETATE/CN
E30          1    ADENOSINE, 2,8-DIMETHYL-/CN
E31          1    ADENOSINE, 2,8-DIMETHYL-, 2',3',5'-TRIACETATE/CN
E32          1    ADENOSINE, 2-(((((2-(3,4-DIHYDRO-2(1H)-ISOQUINOLINYL)ETHYL)A
                  MINO)CARBONYL)AMINO)METHYL)-N-(2,2-DIPHENYLETHYL)-/CN
E33          1    ADENOSINE, 2-(((((2-(BIS(1-METHYLETHYL)AMINO)ETHYL)AMINO)CAR
                  BONYL)AMINO)METHYL)-N-(2,2-BIS(3-METHYLPHENYL)ETHYL)-/CN
E34          1    ADENOSINE, 2-(((((2-(BIS(1-METHYLETHYL)AMINO)ETHYL)AMINO)CAR
                  BONYL)AMINO)METHYL)-N-(2,2-BIS(4-METHYLPHENYL)ETHYL)-/CN
E35          1    ADENOSINE, 2-(((((2-(BIS(1-METHYLETHYL)AMINO)ETHYL)AMINO)CAR
                  BONYL)AMINO)METHYL)-N-(2,2-DIPHENYLETHYL)-/CN
E36          1    ADENOSINE, 2-(((((2-(BIS(1-METHYLETHYL)AMINO)ETHYL)AMINO)CAR
                  BONYL)AMINO)METHYL)-N-(9H-FLUOREN-9-YLMETHYL)-/CN

=> b caplus
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                     ENTRY    SESSION
FULL ESTIMATED COST                                   9.56      11.04

FILE 'CAPLUS' ENTERED AT 08:44:54 ON 12 NOV 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)
```



```
FILE COVERS 1907 - 12 Nov 2010  VOL 153 ISS 21
FILE LAST UPDATED: 11 Nov 2010  (20101111/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED:  Aug 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE:  Aug 2010

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2010.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l3
L4           2 L3

=> d l4 1-2 ibib abs hitstr
```

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1975:108128 CAPLUS
DOCUMENT NUMBER: 82:108128
ORIGINAL REFERENCE NO.: 82:17263a,17266a
TITLE: Correlation between structure and activity with purine derivatives as inhibitors of the adenine phosphoribosyl-transferase
AUTHOR(S): Martin, Miguel; Carbo, Ramon
CORPORATE SOURCE: Dep. Quim. Org., Inst. Quim. Sarria, Barcelona, Spain
SOURCE: Afinidad (1974), 31(320), 757-8
CODEN: AFINAE; ISSN: 0001-9704
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
AB Following a methodol. previously proposed within the framework of Del Re, G. (1958) and HMO (MO) methods, the relation between the adenine phosphoribosyltransferase inhibitory activity and the electronic structure for a family of purine derivs. was studied.
IT ***5327-19-5***
RL: BIOL (Biological study)
(adenine phosphoribosyltransferase inhibition by, structure in relation to)
RN 5327-19-5 CAPLUS
CN 9H-Purine, 2,6-dimethoxy- (CA INDEX NAME)




OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

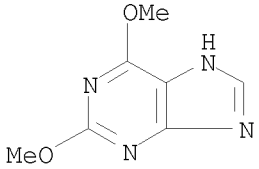
L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1955:69113 CAPLUS
DOCUMENT NUMBER: 49:69113
ORIGINAL REFERENCE NO.: 49:13256a-g
TITLE: Purines. III. The preparation of certain purine and triazolopyrimidine derivatives
AUTHOR(S): Dille, K. L.; Christensen, B. E.
CORPORATE SOURCE: Oregon State Coll., Corvallis
SOURCE: Journal of the American Chemical Society (1954), 76, 5087-8
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C.A. 48, 685f. A series of new purine derivs. and their azapurine analogs has been prepared from 2,6-dichloro-4-amino-5-nitropyrimidine (I). I (5.0 g.) in 110 cc. cold absolute MeOH slowly added during 0.5 hr. at 15-20° to 1.1 g. Na in 50 cc. absolute MeOH, and the mixture stirred 3 hrs., boiled 3 min., and cooled gave 3.85 g. 2,6-di-MeO analog (II) of I, white needles, m. 180-1° (from aqueous MeOH). I (5.0 g.) in 110 cc. MeOH gave similarly with 1.21 g. Na in 50 cc. MeOH and 4 cc. MeSH 5.2 g. 2,6-di-MeS analog (III) of I, yellow powder, m. 220-1° (from aqueous MeOH). II (1.78 g.) in 160 cc. MeOH hydrogenated over 2 g. Raney Ni at atmospheric pressure yielded 0.7 g. 2,6-dimethoxy-4,5-diaminopyrimidine (IV),

white crystals, m. 177.5-8.5° (from H2O); became discolored on standing. III (2 g.) in 150 cc. MeOH hydrogenated at 24 lb. pressure over Raney Ni yielded 1.5 g. 2,6-di-MeS analog (V) of IV, white shiny flakes, m. 192-3° (from MeOH). II (1.55 g.) in 80 cc. MeOH hydrogenated at 1 atmospheric over Raney Ni, the mixture adjusted to pH 1 with concentrated H2SO4 and cooled, the white crystalline sulfate (1.5 g.) heated 20 min. with 20 cc. HCONH2, cooled, diluted with 10 cc. H2O, and adjusted to pH 7-8, and the mixture refrigerated overnight gave 0.3 g. 2,6-dimethoxypurine, decomposed at 300° and melted at 233° forming a solid-liquid phase up to 300°. IV (1.5 g.) in 45 cc. 5% H2SO4, the solution cooled, the resulting sulfate (1.72 g.) dissolved in 18 cc. hot HCONH2, the solution boiled gently 20-5 min., cooled, diluted with 10 cc. H2O, and let stand overnight gave 1.13 g. 2,6-dimethylmercaptopurine, greenish powder, m. 253-4° with softening at 217°. I (1.0 g.) heated 2.5 hrs. on the steam bath with 4.6 g. NaSH in 50 cc. H2O saturated with H2S, the mixture filtered and acidified with glacial AcOH, and the precipitate recrystd. from 400 cc. H2O yielded 0.6 g. 2,6-di-HS analog (VI) of IV, golden crystals, VI (3.5 g.) refluxed 15 min. in 100 cc. 90% HCO2H yielded 31 g. crude formyl derivative (V). V (2.85 g.) in 29 cc. HCONH2 boiled gently 15 min. and filtered, and the filtrate diluted with 10 cc. H2O and acidified with glacial AcOH yielded 2.52 g. yellow product which twice dissolved in 90 cc. NH4OH, treated with Norit, and repptd. with AcOH yielded 2.22 g. 2,6-dimercaptopurine, yellow powder. VI (0.8 g.) in 500 cc. H2O containing 0.3 cc. concentrated H2SO4 decolorized with Norit, treated with stirring at 10° with 0.4 g. NaNO2 and stirred 1 hr. gave 0.58 g. 5,7-dimercapto-1H-γ-triazolo[d]pyrimidine (VII), exploded on rapid heating, and gradually turned brown when heated up to 300°. V (0.6 g.) in 350 cc. hot H2O containing 0.2 cc. concentrated H2SO4 cooled to 15°, filtered, treated with stirring with 0.3 g. NaNO2, stirred 0.5 hr., and cooled 2 hrs. gave 0.59 g. 5,7-dimethylmercapto analog of VII, white powder, m. 228-9° (from MeOH). IV sulfate (1.5 g.) in 100 cc. boiling H2O treated at 10° with 0.42 g. NaNO2 gave similarly 0.88 g. 5,7-di-MeO analog of VII, white powder, m. 215-16° (from MeOH). 2-Mercapto-4,5-diaminopyrimidine (2.0 g.) dissolved in 1200 cc. H2O containing 0.2 g. NaNO2, the solution decolorized with Norit and filtered, the filtrate acidified at 30° dropwise with AcOH to pH 5-6 and let stand overnight, and the crude solid (1.6 g.) dissolved in 50 cc. dilute NH4OH and repptd. with AcOH gave 5-mercapto-1H-γ-triazolo[d]pyrimidine, exploded on a m.p. block.

IT ***5327-19-5P***, Purine, 2,6-dimethoxy-
RL: PREP (Preparation)
(preparation of)

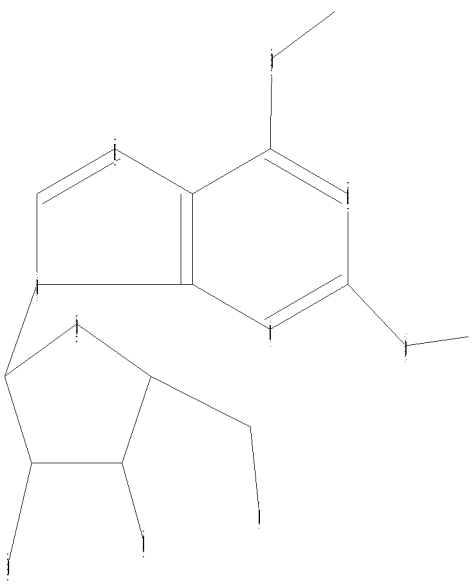
RN 5327-19-5 CAPLUS

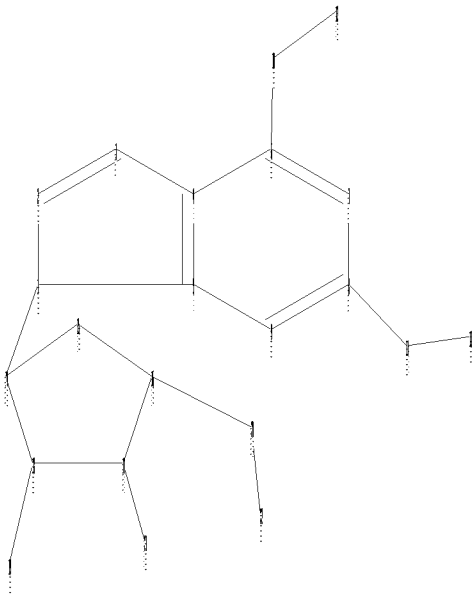
CN 9H-Purine, 2,6-dimethoxy- (CA INDEX NAME)




OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

```
=> FIL STNGUIDE
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                    12.62      23.66

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                    -1.70      -1.70

FILE 'STNGUIDE' ENTERED AT 08:45:48 ON 12 NOV 2010
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Nov  5, 2010 (20101105/UP).

=> b reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                     0.21      23.87

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -1.70

FILE 'REGISTRY' ENTERED AT 08:47:25 ON 12 NOV 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2010 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   11 NOV 2010  HIGHEST RN 1252761-16-2
DICTIONARY FILE UPDATES:  11 NOV 2010  HIGHEST RN 1252761-16-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\jlau1\My Documents\10581544 -
spongosine\reagent 2.str
```





chain nodes :
10 11 12 13 19 20 21 22
ring nodes :
1 2 3 4 5 6 7 8 9 14 15 16 17 18
chain bonds :
1-14 6-10 8-11 10-12 11-13 16-20 17-21 18-19 20-22
ring bonds :
1-2 1-5 2-3 3-4 4-5 4-6 5-9 6-7 7-8 8-9 14-15 14-18 15-16 16-17 17-18

exact/norm bonds :
1-2 1-5 1-14 2-3 3-4 6-10 8-11 10-12 11-13 14-15 14-18 15-16 16-17
17-18 17-21 18-19 20-22
exact bonds :
16-20
normalized bonds :
4-5 4-6 5-9 6-7 7-8 8-9

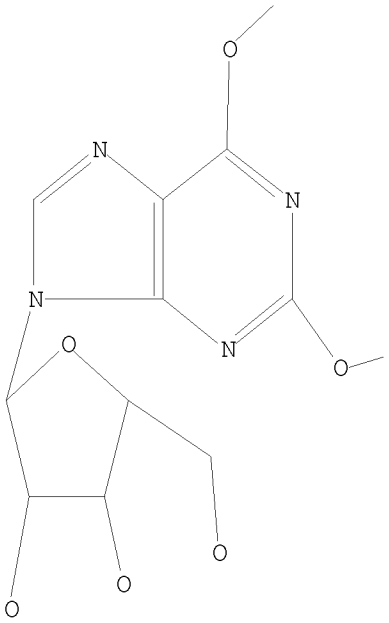
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS
20:CLASS 21:CLASS 22:CLASS

L5 STRUCTURE UPLOADED

=> d l5 sss sam
L5 HAS NO ANSWERS
'SSS SAM ' IS NOT A VALID STRUCTURE FORMAT KEYWORD
ENTER STRUCTURE FORMAT (SIM), NOS:exit
'EXIT' IS NOT A VALID STRUCTURE FORMAT KEYWORD
ENTER STRUCTURE FORMAT (SIM), NOS:quit
'QUIT' IS NOT A VALID STRUCTURE FORMAT KEYWORD
<------User Break------>

ENTER STRUCTURE FORMAT (SIM), NOS:

ENTER STRUCTURE FORMAT (SIM), NOS:
ENTER STRUCTURE FORMAT (SIM), NOS:
ENTER STRUCTURE FORMAT (SIM), NOS:
YOU HAVE RECEIVED THIS PROMPT MESSAGE 5 CONSECUTIVE TIMES WITHOUT ENTERING A REQUESTED RESPONSE
Structure Formats
SIM ----- Structure IMage (no node numbers).
NOS ----- NO Structure data.
IF YOU REQUIRE FURTHER HELP, PLEASE CONTACT YOUR LOCAL HELP DESK
ENTER STRUCTURE FORMAT (SIM), NOS:sim
L5 STR




Structure attributes must be viewed using STN Express query preparation.

=> s l5 sss sam
SAMPLE SEARCH INITIATED 08:48:16 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 28 TO ITERATE

100.0% PROCESSED 28 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

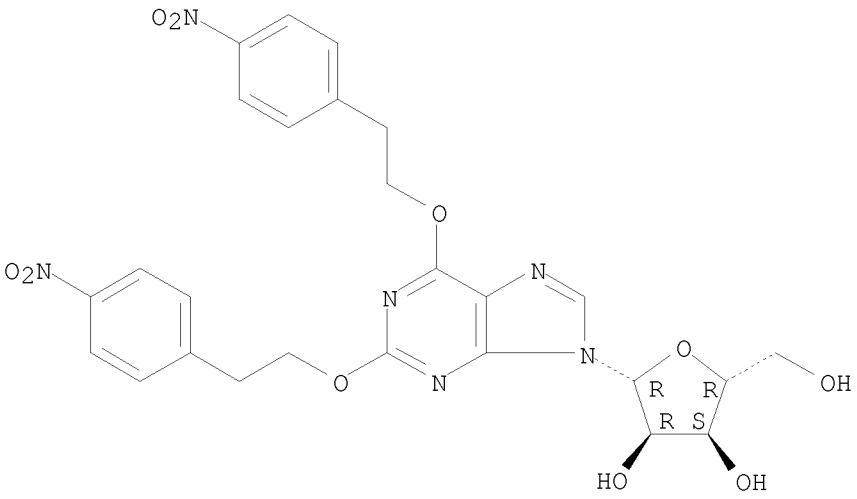
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 243 TO 877
PROJECTED ANSWERS: 1 TO 80

L6 1 SEA SSS SAM L5

=> d l6 scan

L6 1 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN Xanthosine, 2,6-bis-O-[2-(4-nitrophenyl)ethyl]- (9CI)
MF C26 H26 N6 O10

Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

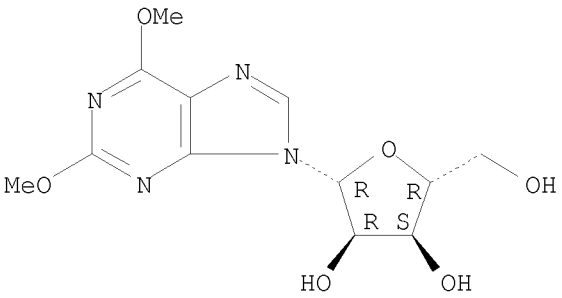
ALL ANSWERS HAVE BEEN SCANNED

```
=> e xanthosine/cn
E1            1     XANTHORRHONE, 14-HYDROXY-/CN
E2            2     XANTHOSIDERITE/CN
E3            1 --> XANTHOSINE/CN
E4            1     XANTHOSINE 3',5'-MONOPHOSPHATE/CN
E5            1     XANTHOSINE 5'-(B,Γ-IMIDO)TRIPHOSPHATE/CN
E6            1     XANTHOSINE 5'-(B,Γ-METHYLENE)TRIPHOSPHATE/CN
E7            1     XANTHOSINE 5'-(PENTAHYDROGEN TETRAPHOSPHATE), P'''.FWDARW.5'
                    -ESTER WITH ADENOSINE/CN
E8            1     XANTHOSINE 5'-(PENTAHYDROGEN TETRAPHOSPHATE), P'''.FWDARW.5'
                    -ESTER WITH URIDINE/CN
E9            1     XANTHOSINE 5'-(PENTAHYDROGEN TETRAPHOSPHATE), P'''.FWDARW.5'
                    -ESTER WITH XANTHOSINE/CN
E10           1     XANTHOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE)/CN
E11           1     XANTHOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE), 2'(OR 3')-(2-(ME
                    THYLAMINO)BENZOATE)/CN
E12           1     XANTHOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE), 2',3'-DIDEOXY-/C
                    N

=> e
E13           1     XANTHOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE), 2',3'-DIDEOXY-8-
                    METHYL-/CN
E14           1     XANTHOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE), 2'-DEOXY-/CN
E15           1     XANTHOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE), 6-THIO-/CN
E16           1     XANTHOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE), CHROMIUM COMPLEX
                    /CN
E17           1     XANTHOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE), DISODIUM SALT/CN
E18           1     XANTHOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE), MAGNESIUM SALT (
                    1:1)/CN
E19           1     XANTHOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE), P''-ETHYL ESTER/
                    CN
E20           1     XANTHOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE), P''.FWDARW.5'-ES
                    TER WITH ADENOSINE/CN
```

```
E21          1     XANTHOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE), P''.FWDARW.5'-ES
                   TER WITH URIDINE/CN
E22          1     XANTHOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE), P''.FWDARW.5'-ES
                   TER WITH XANTHOSINE/CN
E23          1     XANTHOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE), TRISODIUM SALT/C
                   N
E24          1     XANTHOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE-P',P''-32P2)/CN

=> e
E25          1     XANTHOSINE 5'-(TRIHYDROGEN DIPHOSPHATE)/CN
E26          1     XANTHOSINE 5'-(TRIHYDROGEN DIPHOSPHATE), 2'(OR 3')-(2-(METHY
                   LAMINO)BENZOATE)/CN
E27          1     XANTHOSINE 5'-(TRIHYDROGEN DIPHOSPHATE), 2',3'-DIDEOXY-8-MET
                   HYL-/CN
E28          1     XANTHOSINE 5'-(TRIHYDROGEN DIPHOSPHATE), 2,6-DI-S-METHYL-2,6
                   -DITHIO-/CN
E29          1     XANTHOSINE 5'-(TRIHYDROGEN DIPHOSPHATE), 2-DEOXY-/CN
E30          1     XANTHOSINE 5'-(TRIHYDROGEN DIPHOSPHATE), 2-S-METHYL-2-THIO-/
                   CN
E31          1     XANTHOSINE 5'-(TRIHYDROGEN DIPHOSPHATE), 2-S-METHYL-2-THIO-,
                    P'-(2-(TRIMETHYLAMMONIO)ETHYL) ESTER, INNER SALT/CN
E32          1     XANTHOSINE 5'-(TRIHYDROGEN DIPHOSPHATE), 6-THIO-/CN
E33          1     XANTHOSINE 5'-(TRIHYDROGEN DIPHOSPHATE), 7-B-D-RIBOFURA
                   NOSYL-, INNER SALT, INTRAMOL. P',5''-ESTER/CN
E34          1     XANTHOSINE 5'-(TRIHYDROGEN DIPHOSPHATE), 7-METHYL-, INNER SA
                   LT/CN
E35          1     XANTHOSINE 5'-(TRIHYDROGEN DIPHOSPHATE), DISODIUM SALT/CN
E36          1     XANTHOSINE 5'-(TRIHYDROGEN DIPHOSPHATE), P'-(2,3,4-TRI-O-ACE
                   TYL-6-DEOXY-B-L-GALACTOPYRANOSYL) ESTER/CN

=> e xanthosine, 2,6-/cn
E1           1     XANTHOSINE, 2'-O-PICRYL-/CN
E2           1     XANTHOSINE, 2,2',3',5',6-PENTAKIS-O-(TRIMETHYLSILYL)-/CN
E3           0 --> XANTHOSINE, 2,6-/CN
E4           1     XANTHOSINE, 2,6-BIS-O-(2-(4-NITROPHENYL)ETHYL)-/CN
E5           1     XANTHOSINE, 2,6-BIS-S-(PHENYLMETHYL)-2,6-DITHIO-/CN
E6           1     XANTHOSINE, 2,6-DI-O-ETHYL-/CN
E7           1     XANTHOSINE, 2,6-DI-O-METHYL-/CN
E8           1     XANTHOSINE, 2,6-DI-S-METHYL-2,6-DITHIO-/CN
E9           1     XANTHOSINE, 2,6-DI-S-METHYL-2,6-DITHIO-, 2',3',5'-TRIACETATE
                   /CN
E10          1     XANTHOSINE, 2,6-DI-SE-METHYL-2,6-DISELENO-/CN
E11          1     XANTHOSINE, 2,6-DITHIO-/CN
E12          1     XANTHOSINE, 2,6-DITHIO-, 2',3',5'-TRIACETATE/CN

=> s e7
L7           1 "XANTHOSINE, 2,6-DI-O-METHYL-"/CN

=> d l7

L7   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2010 ACS on STN
RN   88508-72-9  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   Xanthosine, 2,6-di-O-methyl- (9CI)  (CA INDEX NAME)
OTHER NAMES:
CN   2,6-Di-O-methylxanthosine
CN   NSC 31145
FS   STEREOSEARCH
MF   C12 H16 N4 O6
```

LC  STN Files:  BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL
        (*File contains numerically searchable property data)

Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> b caplus

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 9.56 | 33.43 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | 0.00 | -1.70 |

FILE 'CAPLUS' ENTERED AT 08:50:01 ON 12 NOV 2010


FILE COVERS 1907 - 12 Nov 2010  VOL 153 ISS 21
FILE LAST UPDATED: 11 Nov 2010  (20101111/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED:  Aug 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE:  Aug 2010

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2010.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.

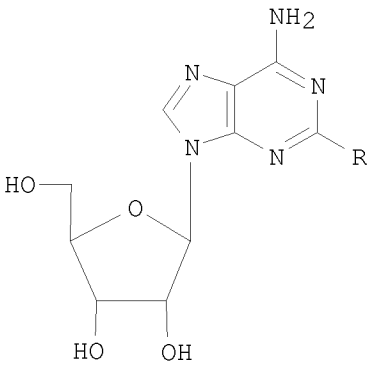
=> s l7
L8 4 L7

=> d l8 1-4 ibib abs hitstr

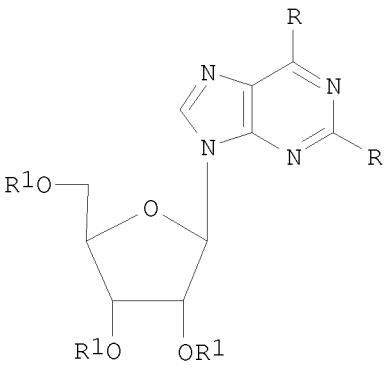
L8 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:523477 CAPLUS
DOCUMENT NUMBER: 143:7942
TITLE: Improved synthesis of 2-substituted adenosines
INVENTOR(S): Savory, Edward Daniel
PATENT ASSIGNEE(S): Cambridge Biotechnology Limited, UK
SOURCE: PCT Int. Appl., 24 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2005054269 | A1 | 20050616 | WO 2004-GB5092 | 20041203 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| AU 2004295172 | A1 | 20050616 | AU 2004-295172 | 20041203 |
| CA 2552591 | A1 | 20050616 | CA 2004-2552591 | 20041203 |
| EP 1697393 | A1 | 20060906 | EP 2004-805920 | 20041203 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS | | | | |
| CN 1886415 | A | 20061227 | CN 2004-80035593 | 20041203 |
| CN 100532389 | C | 20090826 | | |
| JP 2007513135 | T | 20070524 | JP 2006-542019 | 20041203 |
| NZ 546781 | A | 20100226 | NZ 2004-546781 | 20041203 |
| NO 2006003112 | A | 20060905 | NO 2006-3112 | 20060704 |
| KR 2006125829 | A | 20061206 | KR 2006-7013387 | 20060704 |
| IN 2006CN02453 | A | 20070608 | IN 2006-CN2453 | 20060705 |
| HK 1097850 | A1 | 20100409 | HK 2007-104299 | 20070424 |
| US 20080262214 | A1 | 20081023 | US 2008-581544 | 20080708 |
| PRIORITY APPLN. INFO.: | | | GB 2003-28323 A | 20031205 |
| | | | WO 2004-GB5092 W | 20041203 |

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 143:7942; MARPAT 143:7942
GI



I



II

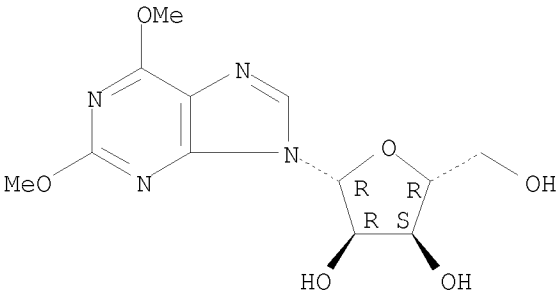
AB A method of synthesis of a 2-substituted adenosine I which comprises converting a compound of formula II via aminolysis reaction, wherein R is alkoxy, benzoyl, or phenoxy groups (unsubstituted, or mono-, or di-substituted by halo, amino, CF3-, cyano, nitro, alkyl, alkoxy); R1 = H, or a protecting group. Thus, I (R = OMe) was prepd,. from inosine via aminolysis reaction.

IT ***88508-72-9P***
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(improved synthesis of spongosine from inosine via aminolysis reaction)

RN 88508-72-9 CAPLUS

CN Xanthosine, 2,6-di-O-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2001:367014 CAPLUS

DOCUMENT NUMBER: 135:211207

TITLE: Influence of methylation and interactions with amino acid carboxylic groups on the UV spectra of purine bases and nucleosides in dimethyl sulfoxide. 3. Hypoxanthine and xanthine

AUTHOR(S): Stepanyugin, A. V.; Kolomiets, I. M.; Potyagailo, A. L.; Trigubenko, S. A.; Bogdan, T. V.; Samiilenko, S. P.

CORPORATE SOURCE: Inst. Molekulyarnoi Biol. i Genetiki, NAN Ukraini, Kiev, 03143, Ukraine

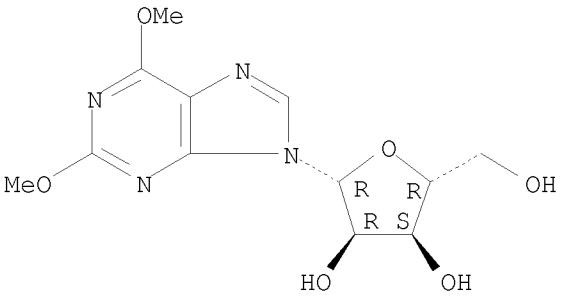
SOURCE: Biopolimeri i Klitina (2001), 17(1), 43-60

CODEN: BKILAK
PUBLISHER: Institut Molekulyarnoi Biologii i Genetiki NAN Ukraini
DOCUMENT TYPE: Journal
LANGUAGE: Ukrainian

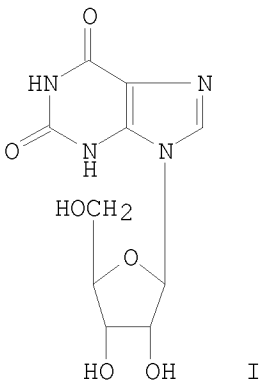
AB UV absorption spectra of hypoxanthine, xanthine, their nucleosides and a number of their Me derivs. were studied in anhydrous DMSO, and the spectral changes under the interaction with neutral and deprotonated (carboxylate-ion) amino acid carboxylic group were traced. By the semi-empirical quantum-chemical method MNDO/H it was shown, that the interaction with carboxylate-ion fixes Hyp in the rare enolic form and shifts the N7H ↔ N9H tautomeric equilibrium to the left while in the case of Xan provokes the N7H → N9H transition, which is blocked up by its Me substitution at the position N3. Significant changes in the UV spectra of Xan, m3Xan, m9Xan and X under the interaction with carboxylate-ion are determined by the essential contribution to a complex formation of the proton transfer from a base to the ligand, m9Xan and X proving to be partly deprotonated even on the account of the solvent. It was established that Me substitution at the position N7 in m7I and m7X resulted in the practical absence of their interaction with carboxylate-ion and the rise of a new ability of forming complexes with the neutral carboxylic group. The substitution of the C8H group for N in 8-azaXan does not change the interaction specificity of this base with tow forms of carboxylic group.

IT ***88508-72-9***, 2,6-Di-O-methylxanthosine
RL: PRP (Properties)
(interactions of hypoxanthine, xanthine, inosine and xanthosine Me derivs. with amino acids by UV absorption)
RN 88508-72-9 CAPLUS
CN Xanthosine, 2,6-di-O-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




L8 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1984:68638 CAPLUS
DOCUMENT NUMBER: 100:68638
ORIGINAL REFERENCE NO.: 100:10469a,10472a
TITLE: Tautomerism and ionization of xanthosine
AUTHOR(S): Roy, Kunal B.; Miles, H. Todd
CORPORATE SOURCE: Lab. Mol. Biol., Natl. Inst. Arthritis, Diabetes, Dig. Kidney Dis., Bethesda, MD, 20205, USA
SOURCE: Nucleosides & Nucleotides (1983), 2(3), 231-42
CODEN: NUNUD5; ISSN: 0732-8311
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

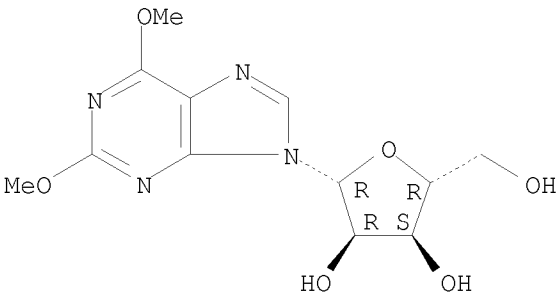
AB Tautomerism and ionization of xanthosine (I) were studied by IR spectroscopy. N-Me and O-Me model compds., which are isoelectronic with possible keto and enol tautomers were prepared, and comparison of their spectra with neutral and with ionized I showed that unionized I has the diketo structure and that on acid dissociation (pK 5.7), the 1st proton is lost from N-3 (rather than N-1) to give the 6-keto-2-enolate anion. Specific labeling at the 2- and 6-positions with 18O confirmed these conclusions. The close similarity of the IR spectra of poly(xanthylic acid) (II) to those of the monomers and model compds. show that II has the diketo structure below pH .apprx.5 and the 6-keto-2-enolate anion structure at neutral and slightly basic pH.

IT ***88508-72-9P***
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and IR spectra of, tautomerism of xanthosine in relation to)

RN 88508-72-9 CAPLUS

CN Xanthosine, 2,6-di-O-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



OS.CITING REF COUNT: 22 THERE ARE 22 CAPLUS RECORDS THAT CITE THIS RECORD (22 CITINGS)

L8 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1959:11835 CAPLUS

DOCUMENT NUMBER: 53:11835

ORIGINAL REFERENCE NO.: 53:2236a-i,2237a

TITLE: Synthesis of potential anticancer agents. XIV. Ribosides of 2,6-disubstituted purines

AUTHOR(S): Schaeffer, Howard J.; Thomas, H. Jeanette

CORPORATE SOURCE: Southern Research Inst., Birmingham, AL

SOURCE: Journal of the American Chemical Society (1958), 80, 3738-42
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 53:11835

AB cf. C.A. 52, 10104e. 2,6-Dichloropurine (1.60 g.), 2.40 g. Celite, 1.14 g. $HgCl_2$, and 210 cc. 50% aqueous EtOH treated slowly with stirring with 3.04 cc. 10% aqueous NaOH, cooled overnight, and filtered, and the residue washed and dried 8 hrs. at 61°/3 mm. over $P_2O_5$ yielded 4.80 g. mixture of 2.40 g. Celite and 2.40 g. bis(2,6-dichloropurinyl)mercury (I). 2,3,5-Tri-O-benzoyl-D-ribofuranosyl chloride from 7.67 g. 1-O-acetyl-2,3,5-tri-O-benzoyl-β-ribose in 50 cc. xylene added to 4.38 g. I and 4.60 g. Celite in 400 cc. dry xylene, refluxed 2 hrs. with stirring and filtered, the filter cake washed with hot $CHCl_3$, the xylene filtrate evaporated, the residue dissolved in hot $CHCl_3$, and the combined $CHCl_3$ solns. washed with 30% aqueous KI and $H_2O$, dried, treated with C, and concentrated yielded 9.93 g. 2,6-dichloro-9-(2,3,5-tri-O-benzoyl)-β-D-ribofuranosylpurine (II), tan glass. Crude II (2.11 g.) in 100 cc. absolute MeOH refluxed 1 hr., neutralized with AcOH, and evaporated in vacuo, the residue dissolved in 30 cc. $H_2O$ and extracted with $CHCl_3$, the aqueous solution evaporated to leave 800 mg. gel, and a 200-mg. portion subjected to a partition chromatography on Celite with $H_2O$-saturated BuOH yielded 140 mg. 2-chloro-6-methoxy-9-β-D-ribofuranosylpurine (III), m. 140° (iso-PrOH-EtOAc), $[\alpha]_D^{26}$ -30.4 ± 2.3° (c 0.612, MeOH). III (308 mg.) in 50 cc. 50% aqueous MeOH hydrogenated under ambient conditions 39 min. over 100 mg. 5% Pd-C and 40 mg. MgO gave 203 mg. 6-methoxy-9-β-D-ribofuranosylpurine, m. 140° (MeOH-EtOAc). III (176 mg.) in 15 cc. MeOH (saturated with $NH_3$ at 0°) heated 16 hrs. at 83° in a steel bomb, filtered, and evaporated in vacuo, the residue dissolved in $H_2O$, the solution treated with 10 cc. 14% aqueous picric acid, the precipitate filtered off and dissolved in $H_2O$, the aqueous solution stirred with 0.3 g. Dowex 1 ($CO_3$) and filtered, and the filtrate evaporated yielded 61 mg. 6-amino-2-chloro-9-β-D-ribofuranosylpurine (IV), m. 145-6° (decomposition). III (500 mg.) in 75 cc. MeOH treated with 3.16 cc. N NaSMe in MeOH, refluxed 2 hrs., cooled, neutralized with N HCl, and evaporated in vacuo, and the residue dissolved in hot $H_2O$ and cooled yielded 203 mg. amorphous 2-MeS analog of III, m. 160-1° with softening at 116°, $[\alpha]_D^{26}$ -16.9 ± 2.1° (c 0.649, MeOH); 2nd crop, 140 mg. III (500 mg.) in 75 cc. MeOH refluxed 4 hrs. with 3.16 cc. N NaOMe, neutralized with N HCl, and evaporated in vacuo, and the residue recrystd. from $H_2O$ and dried 24 hrs. at 110°/0.08 mm. over $P_2O_5$ gave 155 mg. 2,6-dimethoxy-9-β-D-ribofuranosylpurine, m. 163° with softening at 120°, $[\alpha]_D^{32}$ -33.6 ± 2.2° (c 0.648, MeOH). Crude II (6.00 g.) and 420 cc. MeOH (saturated at 0° with $NH_3$) stirred to solution, kept overnight, and evaporated in vacuo, the residue dissolved in 40 cc. $H_2O$, washed with $CHCl_3$, treated with 25 cc. 11% aqueous picric acid, and filtered, the residue dissolved in $H_2O$, the solution stirred with 9 g. Dowex 1 ($CO_3$) resin and filtered, and the filtrate concentrated to 20 cc. gave 670 mg. IV, m. 142° (decomposition). IV (302 mg.) in 50 cc. MeOH refluxed 16 hrs. with 2 cc. N NaOMe, cooled, neutralized with N HCl, and evaporated in vacuo, and the residue recrystd. from $H_2O$ yielded 104 mg. 2-MeO analog of IV, m. 190-2° (decomposition), $[\alpha]_D^{26}$ -43.3 ± 2.3° (c 0.610, MeOH). IV (300 mg.) in 50 cc. PrOH treated with 2.0 cc. N NaSMe in PrOH, refluxed 2.5 hrs., neutralized with N HCl, and filtered, and the filtrate evaporated in vacuo

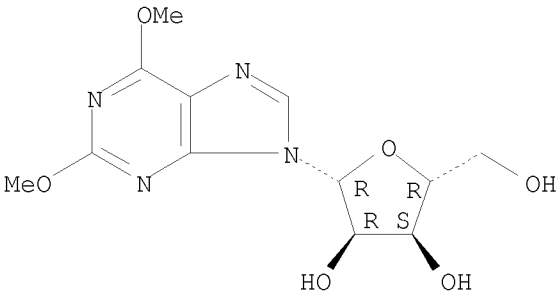
yielded 119 mg. 2-MeS analog of IV, m. 153° resolidified 185-90° and remelted 220° (decomposition). IV (302 mg.) in 10 cc. 25% aqueous Me2NH diluted with 35 cc. MeOH, heated 16 hrs. in a bomb at 100°, and evaporated in vacuo, and the residue crystallized from 40 cc. H2O yielded 221 mg. 2-Me2N analog of IV, m. 213° (decomposition). IV (302 mg.) in 10 cc. 40% aqueous MeNH2 diluted with 35 cc. MeOH and heated 4 hrs. in a bomb at 100°, the solution evaporated to dryness, and the residue crystal. from MeOH-EtOAc yielded 116 mg. 2-MeNH analog of IV, m. 198° (decomposition), [α]26D -42.8 ± 3.3° (c 0.416, MeOH). IV (602 mg.) added in portions to 30 cc. N2H4, kept 16 hrs. at room temperature under N, and evaporated in vacuo at 30°, and the residue evaporated 3 times with 15-cc. portions iso-PrOH and recrystd. yielded 225 mg. 2-H2NNH analog (V) of IV, m. 143° resolidified at 150-5° and remelted at 200° with decomposition (2nd crop, 51 mg.), [α]26D -33.0 ± 1.8° (c 0.763, H2O). V (297 mg.) in 7 cc. 5% aqueous AcOH treated with cooling with 83 mg. NaNO2 in 17 cc. H2O, cooled 1 hr., and filtered, and the residue (218 mg.) recrystd. from H2O and dried 48 hrs. at 100°/0.07 mm. over P2O5 yielded 142 mg. 2-N2 analog of IV, m. 159-60° (decomposition), [α]26D -27.6 ± 5.8° (c 0.232, MeOH).

IT ***88508-72-9P***, 9H-Purine, 2,6-dimethoxy-9-β-D-ribofuranosyl-
RL: PREP (Preparation)
(preparation of)

RN 88508-72-9 CAPLUS

CN Xanthosine, 2,6-di-O-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)

=> logoff hold

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 23.74 | 57.17 |

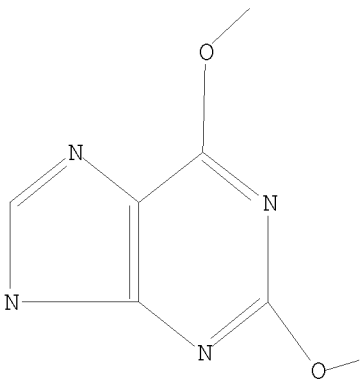
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | -3.40 | -5.10 |

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 08:50:16 ON 12 NOV 2010

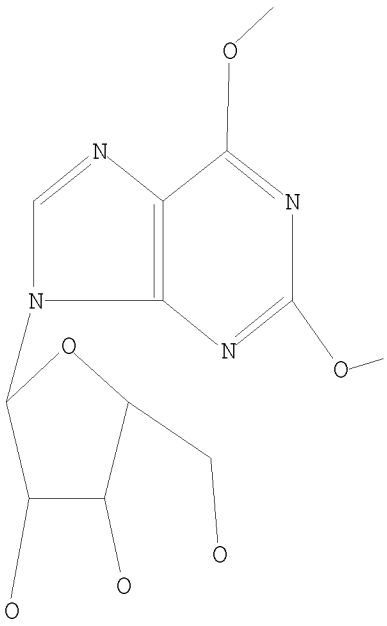
Connecting via Winsock to STN

```
Welcome to STN International!  Enter x:x

LOGINID:ssptajsl1623

PASSWORD:
 * * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 08:59:30 ON 12 NOV 2010
FILE 'CAPLUS' ENTERED AT 08:59:30 ON 12 NOV 2010
COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                      23.74      57.17

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                      -3.40      -5.10

=> d his

     (FILE 'HOME' ENTERED AT 08:38:27 ON 12 NOV 2010)

     FILE 'REGISTRY' ENTERED AT 08:38:42 ON 12 NOV 2010
                E ADENOSINE, 4,6-DIMETHOXY/CN
                E PURINE, 4,6-DIMETHOXY/CN

     FILE 'STNGUIDE' ENTERED AT 08:39:46 ON 12 NOV 2010

     FILE 'REGISTRY' ENTERED AT 08:42:20 ON 12 NOV 2010
L1              STRUCTURE UPLOADED
L2            5 S L1 SSS SAM
                E 9H-PURINE, 2,6-DIMETHOXY/CN
L3            1 S E4
                E ADENOSINE, 2,6-DIMETHOXY-/CN

     FILE 'CAPLUS' ENTERED AT 08:44:54 ON 12 NOV 2010
L4            2 S L3

     FILE 'STNGUIDE' ENTERED AT 08:45:48 ON 12 NOV 2010

     FILE 'REGISTRY' ENTERED AT 08:47:25 ON 12 NOV 2010
L5              STRUCTURE UPLOADED
L6            1 S L5 SSS SAM
                E XANTHOSINE/CN
                E XANTHOSINE, 2,6-/CN
L7            1 S E7

     FILE 'CAPLUS' ENTERED AT 08:50:01 ON 12 NOV 2010
L8            4 S L7

=> d l1
L1 HAS NO ANSWERS
L1              STR
```




Structure attributes must be viewed using STN Express query preparation.

=> d l5
L5 HAS NO ANSWERS
L5 STR




Structure attributes must be viewed using STN Express query preparation.

=> logoff hold

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 24.24 | 57.67 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | -3.40 | -5.10 |

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 08:59:49 ON 12 NOV 2010

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptajsl1623

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

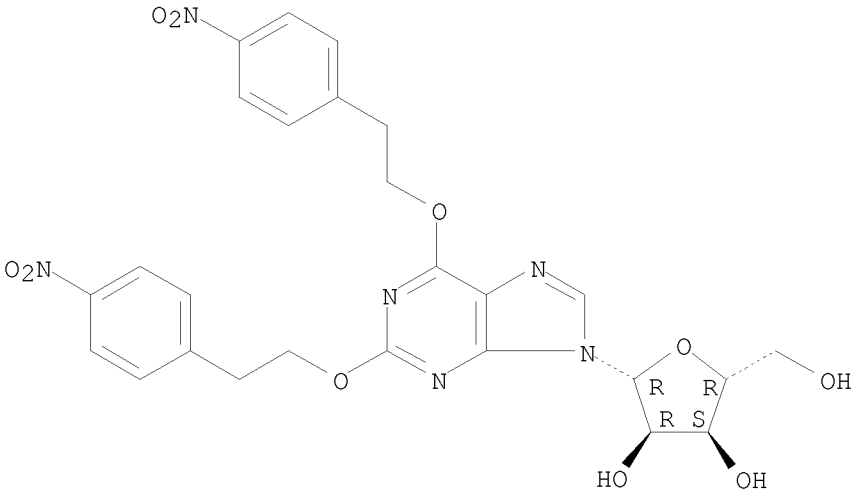
| | | |
|---|---|---|
| NEWS 1 | | Web Page for STN Seminar Schedule - N. America |
| NEWS 2 | APR 02 | CAS Registry Number Crossover Limits Increased to 500,000 in Key STN Databases |
| NEWS 3 | APR 02 | PATDPAFULL: Application and priority number formats enhanced |
| NEWS 4 | APR 02 | DWPI: New display format ALLSTR available |
| NEWS 5 | APR 02 | New Thesaurus Added to Derwent Databases for Smooth Sailing through U.S. Patent Codes |
| NEWS 6 | APR 02 | EMBASE Adds Unique Records from MEDLINE, Expanding Coverage back to 1948 |
| NEWS 7 | APR 07 | 50,000 World Traditional Medicine (WTM) Patents Now Available in CAplus |
| NEWS 8 | APR 07 | MEDLINE Coverage Is Extended Back to 1947 |
| NEWS 9 | JUN 16 | WPI First View (File WPIFV) will no longer be available after July 30, 2010 |
| NEWS 10 | JUN 18 | DWPI: New coverage - French Granted Patents |
| NEWS 11 | JUN 18 | CAS and FIZ Karlsruhe announce plans for a new STN platform |
| NEWS 12 | JUN 18 | IPC codes have been added to the INSPEC backfile (1969-2009) |
| NEWS 13 | JUN 21 | Removal of Pre-IPC 8 data fields streamline displays in CA/CAplus, CASREACT,and MARPAT |
| NEWS 14 | JUN 21 | Access an additional 1.8 million records exclusively enhanced with 1.9 million CAS Registry Numbers -- EMBASE Classic on STN |
| NEWS 15 | JUN 28 | Introducing "CAS Chemistry Research Report": 40 Years of Biofuel Research Reveal China Now Atop U.S. in Patenting and Commercialization of Bioethanol |
| NEWS 16 | JUN 29 | Enhanced Batch Search Options in DGENE, USGENE, and PCTGEN |
| NEWS 17 | JUL 19 | Enhancement of citation information in INPADOC databases provides new, more efficient competitor analyses |
| NEWS 18 | JUL 26 | CAS coverage of global patent authorities has expanded to 61 with the addition of Costa Rica |
| NEWS 19 | SEP 15 | MEDLINE Cited References provide additional revelant records with no additional searching. |
| NEWS 20 | OCT 04 | Removal of Pre-IPC 8 data fields streamlines displays in USPATFULL, USPAT2, and USPATOLD. |
| NEWS 21 | OCT 04 | Precision of EMBASE searching enhanced with new chemical name field |

```
 NEWS 22  OCT 06  Increase your retrieval consistency with new formats  or
                  for Taiwanese application numbers in CA/CAplus.
 NEWS 23  OCT 21  CA/CAplus kind code changes for Chinese patents
                  increase consistency, save time
 NEWS 24  OCT 22  New version of STN Viewer preserves custom
                  highlighting of terms when patent documents are
                  saved in .rtf format
 NEWS 25  OCT 28  INPADOCDB/INPAFAMDB: Enhancements to the US national
                  patent classification.
 NEWS 26  NOV 03  New format for Korean patent application numbers in
                  CA/CAplus increases consistency, saves time.
 NEWS 27  NOV 04  Selected STN databases scheduled for removal on
                  December 31, 2010

 NEWS EXPRESS FEBRUARY 15 10 CURRENT WINDOWS VERSION IS V8.4.2,
          AND CURRENT DISCOVER FILE IS DATED 07 JULY 2010.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that
specific topic.

  All use of STN is subject to the provisions of the STN customer
  agreement.  This agreement limits use to scientific research.  Use
  for software development or design, implementation of commercial
  gateways, or use of CAS and STN data in the building of commercial
  products is prohibited and may result in loss of user privileges
  and other penalties.

* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 13:32:42 ON 12 NOV 2010

=> b reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.22       0.22

FILE 'REGISTRY' ENTERED AT 13:32:52 ON 12 NOV 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2010 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   11 NOV 2010  HIGHEST RN 1252761-16-2
DICTIONARY FILE UPDATES:  11 NOV 2010  HIGHEST RN 1252761-16-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
```

experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

```
=> e xanthosine, 2,6-/cn
E1            1     XANTHOSINE, 2'-O-PICRYL-/CN
E2            1     XANTHOSINE, 2,2',3',5',6-PENTAKIS-O-(TRIMETHYLSILYL)-/CN
E3            0 --> XANTHOSINE, 2,6-/CN
E4            1     XANTHOSINE, 2,6-BIS-O-(2-(4-NITROPHENYL)ETHYL)-/CN
E5            1     XANTHOSINE, 2,6-BIS-S-(PHENYLMETHYL)-2,6-DITHIO-/CN
E6            1     XANTHOSINE, 2,6-DI-O-ETHYL-/CN
E7            1     XANTHOSINE, 2,6-DI-O-METHYL-/CN
E8            1     XANTHOSINE, 2,6-DI-S-METHYL-2,6-DITHIO-/CN
E9            1     XANTHOSINE, 2,6-DI-S-METHYL-2,6-DITHIO-, 2',3',5'-TRIACETATE
                    /CN
E10           1     XANTHOSINE, 2,6-DI-SE-METHYL-2,6-DISELENO-/CN
E11           1     XANTHOSINE, 2,6-DITHIO-/CN
E12           1     XANTHOSINE, 2,6-DITHIO-, 2',3',5'-TRIACETATE/CN

=> e
E13           1     XANTHOSINE, 2-((CYCLOHEXYLMETHYLENE)HYDRAZONE)/CN
E14           1     XANTHOSINE, 2-HYDRAZONE/CN
E15           1     XANTHOSINE, 2-O-(2-(6-BROMO-1H-INDOL-3-YL)ETHYL)-, HYDRAZONE
                    /CN
E16           1     XANTHOSINE, 2-O-BUTYL-/CN
E17           1     XANTHOSINE, 2-O-BUTYL-, 2',3',5'-TRIACETATE/CN
E18           1     XANTHOSINE, 2-O-METHYL-/CN
E19           1     XANTHOSINE, 2-O-METHYL-, 2',3',5'-TRIACETATE/CN
E20           1     XANTHOSINE, 2-O-METHYL-, O-METHYLOXIME/CN
E21           1     XANTHOSINE, 2-S-((1-OXIDO-2-PYRIDINYL)METHYL)-2-THIO-/CN
E22           1     XANTHOSINE, 2-S-((2-CHLORO-4-NITROPHENYL)METHYL)-2-THIO-/CN
E23           1     XANTHOSINE, 2-S-((2-CHLOROPHENYL)METHYL)-2-THIO-/CN
E24           1     XANTHOSINE, 2-S-((3,5-DINITROPHENYL)METHYL)-2-THIO-/CN

=> s e4,e5, e6,e7,e8,e9
              1 "XANTHOSINE, 2,6-BIS-O-(2-(4-NITROPHENYL)ETHYL)-"/CN
              1 "XANTHOSINE, 2,6-BIS-S-(PHENYLMETHYL)-2,6-DITHIO-"/CN
              1 "XANTHOSINE, 2,6-DI-O-ETHYL-"/CN
              1 "XANTHOSINE, 2,6-DI-O-METHYL-"/CN
              1 "XANTHOSINE, 2,6-DI-S-METHYL-2,6-DITHIO-"/CN
              1 "XANTHOSINE, 2,6-DI-S-METHYL-2,6-DITHIO-, 2',3',5'-TRIACETATE"/C
                N
L1            6 ("XANTHOSINE, 2,6-BIS-O-(2-(4-NITROPHENYL)ETHYL)-"/CN OR "XANTHO
                SINE, 2,6-BIS-S-(PHENYLMETHYL)-2,6-DITHIO-"/CN OR  "XANTHOSINE,
                2,6-DI-O-ETHYL-"/CN OR "XANTHOSINE, 2,6-DI-O-METHYL-"/CN OR "XAN
                THOSINE, 2,6-DI-S-METHYL-2,6-DITHIO-"/CN OR "XANTHOSINE, 2,6-DI-
                S-METHYL-2,6-DITHIO-, 2',3',5'-TRIACETATE"/CN)

=> d l1 scan

L1   6 ANSWERS   REGISTRY  COPYRIGHT 2010 ACS on STN
IN   Xanthosine, 2,6-bis-O-[2-(4-nitrophenyl)ethyl]- (9CI)
MF   C26 H26 N6 O10

Absolute stereochemistry.
```

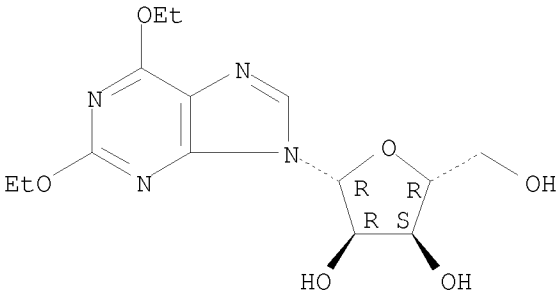


**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L1 6 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN ***Xanthosine, 2,6-di-O-ethyl- (9CI)***
MF C14 H20 N4 O6

Absolute stereochemistry.

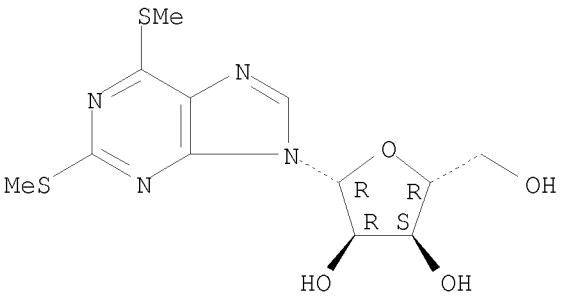


**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L1 6 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN ***Xanthosine, 2,6-di-S-methyl-2,6-dithio- (9CI)***
MF C12 H16 N4 O4 S2

Absolute stereochemistry.

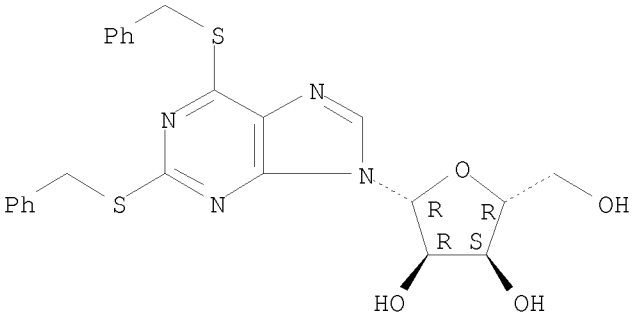



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L1 6 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN ***Xanthosine, 2,6-bis-S-(phenylmethyl)-2,6-dithio- (9CI)***
MF C24 H24 N4 O4 S2

Absolute stereochemistry.

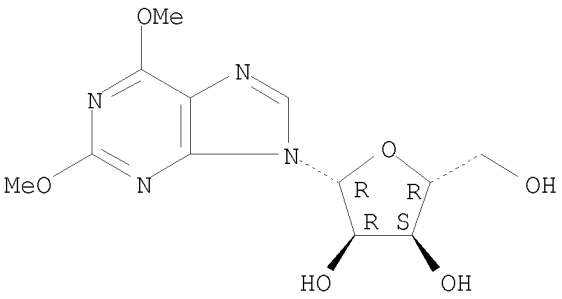



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L1 6 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN ***Xanthosine, 2,6-di-O-methyl- (9CI)***
MF C12 H16 N4 O6

Absolute stereochemistry.

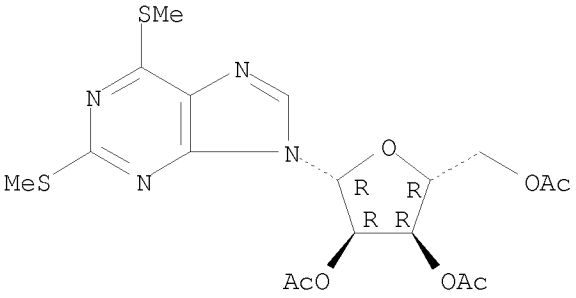



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L1 6 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
IN ***Xanthosine, 2,6-di-S-methyl-2,6-dithio-, 2',3',5'-triacetate (9CI)***
MF C18 H22 N4 O7 S2

Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

ALL ANSWERS HAVE BEEN SCANNED

=> 1
1 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> b caplus

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 33.98 | 34.20 |

FILE 'CAPLUS' ENTERED AT 13:34:15 ON 12 NOV 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.


FILE COVERS 1907 - 12 Nov 2010 VOL 153 ISS 21
FILE LAST UPDATED: 11 Nov 2010 (20101111/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2010

CAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2010.



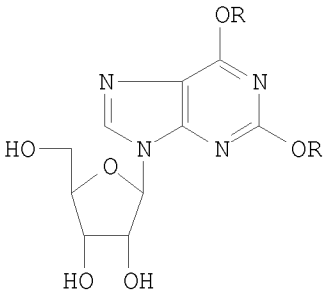
This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s l1
L2          18 L1

=> s l2 and py<= 2003
      24051943 PY<= 2003
L3          17 L2 AND PY<= 2003

=> d l3 1-17 ibib abs
```

L3 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2001:367014 CAPLUS
DOCUMENT NUMBER: 135:211207
TITLE: Influence of methylation and interactions with amino acid carboxylic groups on the UV spectra of purine bases and nucleosides in dimethyl sulfoxide. 3. Hypoxanthine and xanthine
AUTHOR(S): Stepanyugin, A. V.; Kolomiets, I. M.; Potyagailo, A. L.; Trigubenko, S. A.; Bogdan, T. V.; Samiilenko, S. P.
CORPORATE SOURCE: Inst. Molekulyarnoi Biol. i Genetiki, NAN Ukraini, Kiev, 03143, Ukraine
SOURCE: Biopolimeri i Klitina (***2001***), 17(1), 43-60
CODEN: BKILAK
PUBLISHER: Institut Molekulyarnoi Biologii i Genetiki NAN Ukraini
DOCUMENT TYPE: Journal
LANGUAGE: Ukrainian
AB UV absorption spectra of hypoxanthine, xanthine, their nucleosides and a number of their Me derivs. were studied in anhydrous DMSO, and the spectral changes under the interaction with neutral and deprotonated (carboxylate-ion) amino acid carboxylic group were traced. By the

semi-empirical quantum-chemical method MNDO/H it was shown, that the interaction with carboxylate-ion fixes Hyp in the rare enolic form and shifts the N7H ↔ N9H tautomeric equilibrium to the left while in the case of Xan provokes the N7H → N9H transition, which is blocked up by its Me substitution at the position N3. Significant changes in the UV spectra of Xan, m3Xan, m9Xan and X under the interaction with carboxylate-ion are determined by the essential contribution to a complex formation of the proton transfer from a base to the ligand, m9Xan and X proving to be partly deprotonated even on the account of the solvent. It was established that Me substitution at the position N7 in m7I and m7X resulted in the practical absence of their interaction with carboxylate-ion and the rise of a new ability of forming complexes with the neutral carboxylic group. The substitution of the C8H group for N in 8-azaXan does not change the interaction specificity of this base with tow forms of carboxylic group.

L3 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1989:574568 CAPLUS
DOCUMENT NUMBER: 111:174568
ORIGINAL REFERENCE NO.: 111:29091a,29094a
TITLE: Double protection of the heterocyclic base of xanthosine and 2'-deoxyxanthosine
AUTHOR(S): Van Aerschot, A.; Mag, M.; Herdewijn, P.; Vanderhaeghe, H.
CORPORATE SOURCE: Rega Inst., Kathol. Univ., Louvain, B-3000, Belg.
SOURCE: Nucleosides & Nucleotides (***1989***), 8(2), 159-78
CODEN: NUNUD5; ISSN: 0732-8311
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:174568
GI



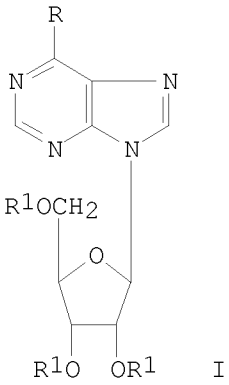

I

AB Reaction of O-protected xanthosines with p-nitrophenylethanol (ROH) under Mitsunobu conditions yields the doubly alkylated O2,O6- (I) and N1-, O2-derivs. Deoxyxanthosine protected on both oxygens with a R group was synthesized starting from deoxyguanosine. Both protecting groups can be eliminated with DBU in pyridine.
OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)

L3 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1988:493494 CAPLUS
DOCUMENT NUMBER: 109:93494
ORIGINAL REFERENCE NO.: 109:15621a,15624a

TITLE: Conformational correlation of purine nucleosides by high-field carbon-13 NMR data
AUTHOR(S): Nair, Vasu; Young, David A.
CORPORATE SOURCE: Dep. Chem., Univ. Iowa, Iowa City, IA, 52242, USA
SOURCE: Magnetic Resonance in Chemistry (***1987***), 25(11), 937-40
CODEN: MRCHEG; ISSN: 0749-1581
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Correlation of the nucleic acid base conformation to 43 purine nucleosides with high-field 13C NMR data is described. A key to the correlation is the chemical shift difference between C-2' and C-3'.
OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD (8 CITINGS)

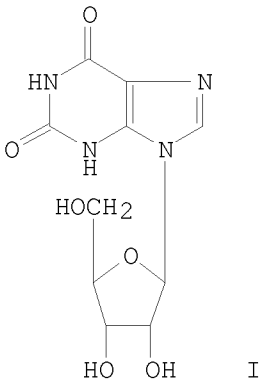
L3 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1986:572916 CAPLUS
DOCUMENT NUMBER: 105:172916
ORIGINAL REFERENCE NO.: 105:27881a,27884a
TITLE: Photoinduced alkylthiolation of halogenated purine nucleosides
AUTHOR(S): Nair, Vasu; Young, David A.
CORPORATE SOURCE: Dep. Chem., Univ. Iowa, Iowa City, IA, 52242, USA
SOURCE: Synthesis (***1986***), (6), 450-3
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:172916
GI



I

AB Five (methylthio)purine nucleosides were prepared from adenosine or guanosine via the title procedure. For example, acetylation of adenosine I (R = NH2, R1 = H) with Ac2O/pyridine gave the triacetate I (R = NH2, R1 = Ac), which was treated with n-pentyl nitrite and CH2I2 in MeCN to give the iodide I (R = iodo, R1 = Ac) (II). Photolysis of the nitrogen-purged solution of II in (MeS)2 with 450 W Hg lamp for 8 h resulted in clean conversion to methylthio derivative I (R = MeS, R1 = Ac; 85% yield) which on deacetylation with NH3/EtOH gave I (R = MeS, R1 = H).
OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

L3 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1984:68638 CAPLUS
DOCUMENT NUMBER: 100:68638
ORIGINAL REFERENCE NO.: 100:10469a,10472a
TITLE: Tautomerism and ionization of xanthosine
AUTHOR(S): Roy, Kunal B.; Miles, H. Todd
CORPORATE SOURCE: Lab. Mol. Biol., Natl. Inst. Arthritis, Diabetes, Dig. Kidney Dis., Bethesda, MD, 20205, USA
SOURCE: Nucleosides & Nucleotides (***1983***), 2(3), 231-42
CODEN: NUNUD5; ISSN: 0732-8311
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

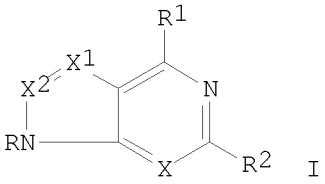


I

AB Tautomerism and ionization of xanthosine (I) were studied by IR spectroscopy. N-Me and O-Me model compds., which are isoelectronic with possible keto and enol tautomers were prepared, and comparison of their spectra with neutral and with ionized I showed that unionized I has the diketo structure and that on acid dissociation (pK 5.7), the 1st proton is lost from N-3 (rather than N-1) to give the 6-keto-2-enolate anion. Specific labeling at the 2- and 6-positions with 18O confirmed these conclusions. The close similarity of the IR spectra of poly(xanthylic acid) (II) to those of the monomers and model compds. show that II has the diketo structure below pH .apprx.5 and the 6-keto-2-enolate anion structure at neutral and slightly basic pH.
OS.CITING REF COUNT: 22 THERE ARE 22 CAPLUS RECORDS THAT CITE THIS RECORD (22 CITINGS)

L3 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1982:45864 CAPLUS
DOCUMENT NUMBER: 96:45864
ORIGINAL REFERENCE NO.: 96:7415a,7418a
TITLE: Pyrazolo[3,4-d]pyrimidine ribonucleosides as anticoccidials. 1. Synthesis and activity of some nucleosides of purines and 4-(alkylthio)pyrazolo[3,4-d]pyrimidines
AUTHOR(S): Krenitsky, Thomas A.; Rideout, Janet L.; Koszalka, George W.; Inmon, Rosetta B.; Chao, Esther Y.; Elion, Gertrude B.; Latter, Victoria S.; Williams, Raymond B.
CORPORATE SOURCE: Wellcome Res. Lab., Research Triangle Park, NC, 27709,

USA
SOURCE: Journal of Medicinal Chemistry (***1982***), 25(1), 32-5
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Thirty-seven purine and pyrazolo[3,4-d]pyrimidine bases and nucleosides I (X, X1, and X2 = CH or N; R = H, ribose, etc.; R1 = H, SMe, SEt, etc; R2 = H, Me, NH2, or SMe), 16 which were synthesized, were tested for anticoccidial activity. 4-(ethylthio)-1-β-D-ribofuranosyl-1H-pyrazol[3,4-d]pyrimidine [77975-21-4], The most active compound in vivo, cleared all chicks of Eimeria tenella lesions when given in the diet at 50 ppm. In vitro, this compound was not cytotoxic to embryonic chick line cells at concns. of 125 mg/L, and in repeated expts., no deaths attributable to toxicity were seen at 400 ppm in the diet. Structure-activity relations are discussed.
OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

L3 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1975:564516 CAPLUS
DOCUMENT NUMBER: 83:164516
ORIGINAL REFERENCE NO.: 83:25831a
TITLE: Adenosine derivatives
INVENTOR(S): Pohlke, Rolf; Mehrhof, Werner; Nowak, Herbert; Simane, Zdenek; Schliep, Jochen; Becker, Karl Heinz
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Fed. Rep. Ger.
SOURCE: Ger. Offen., 16 pp. Addn. to Ger. Offen. 2,230,160.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 2402804 | A1 | 19750731 | DE 1974-2402804 | 19740122 <-- |

PRIORITY APPLN. INFO.: DE 1974-2402804 19740122
AB N6-[(2RS)-1,2,3,4-tetrahydro-2-naphthyl]adenosine, effective in lowering blood lipoprotein levels (no data), was prepared by treatment of RS-2-amino-1,2,3,4-tetrahydronaphthalene with adenosine, or 6-chloro- or 6-(methylmercapto)-9-β-D-ribofuranosylpurine. The 2S or 2R isomers were similarly prepared from the corresponding amines.
OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

L3 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1975:479518 CAPLUS
DOCUMENT NUMBER: 83:79518
ORIGINAL REFERENCE NO.: 83:12499a,12502a
TITLE: Synthesis and coronary vasodilating activity of 2-substituted adenosines
AUTHOR(S): Marumoto, Ryuji; Yoshioka, Yoshio; Miyashita, Osamu; Shima, Shunsuke; Imai, Kinichi; Kawazoe, Katsuyoshi; Honjo, Mikio
CORPORATE SOURCE: Cent. Res. Div., Takeda Chem. Ind., Osaka, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (***1975***), 23(4), 759-74
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 2-Haloadenosines were prepared by acetylation of 2-haloinosines followed by chlorination and amination. 2-Alkoxyadenosines were prepared by protection of 2'- and 3'-OH groups of 2-chloroadenosine (I) or 2-chloroinosine, followed by substitution of the C atom with alkoxy group. The reaction of 5-amino-4-cyano-1-β-D-ribofuranosylimidazole with CS2 afforded 2,6-di-mercapto-9-β-D-ribofuranosylpurine, which was converted to 2-mercaptoadenosine and its S-substituted derivs. 2-Phenylaminoadenosine (II) was prepared from 2-phenylamino-2',3',5'-tri-O-acetylinosine, which was prepared by acetylation of 2-phenylaminoinosine with AcCl in HOAc. O-substituted 2-hydroxyadenosines, S-substituted 2-mercaptoadenosines, N2-substituted 2-aminoadenosines, 2-alkyl- and -aryl-adenosines were prepared among which several compds. had coronary vasodilating potency. II showed not only a strong potency, but also a longer duration of the effect than that of I.

OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)

L3 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1974:108823 CAPLUS
DOCUMENT NUMBER: 80:108823
ORIGINAL REFERENCE NO.: 80:17519a,17522a
TITLE: Lipoprotein level-lowering adenosine derivative
INVENTOR(S): Pohlke, Rolf; Mehrhof, Werner; Becker, Karl Heinz; Schliep, Hans J.; Nowak, Herbert; Simane, Zdenek
PATENT ASSIGNEE(S): Merck Patent G.m.b.H.
SOURCE: Ger. Offen., 16 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 2230160 | A1 | 19740131 | DE 1972-2230160 | 19720621 <-- |
| US 3922261 | A | 19751125 | US 1973-371779 | 19730620 <-- |

PRIORITY APPLN. INFO.: DE 1972-2230160 A 19720621
GI For diagram(s), see printed CA Issue.

AB The adenosine derivative I (R = 1,2,3,4-tetrahydro-2-naphthylamino), useful e.g. for lowering the lipoprotein level in blood, was prepared, e.g. by reaction of I (R = Cl, SMe) optionally containing O-protective groups with 1,2,3,4-tetrahydro-2-naphthylamine.

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L3 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1973:526750 CAPLUS
DOCUMENT NUMBER: 79:126750
ORIGINAL REFERENCE NO.: 79:20586h,20587a
TITLE: Coronary dilating and analgesic adenosine derivatives
INVENTOR(S): Pohlke, Rolf; Jonas, Rochus; Mehrhof, Werner; Schliep, Hans J.; Becker, Karl Heinz; Nowak, Herbert; Simane, Zdenek
PATENT ASSIGNEE(S): Merck Patent G.m.b.H.
SOURCE: Ger. Offen., 54 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 2205002 | A1 | 19730809 | DE 1972-2205002 | 19720203 <-- |
| AU 7240345 | A | 19730927 | AU 1972-40345 | 19720323 <-- |
| NL 7203984 | A | 19721012 | NL 1972-3984 | 19720324 <-- |
| IL 39080 | A | 19750625 | IL 1972-39080 | 19720326 <-- |
| CS 161940 | B2 | 19750610 | CS 1972-88 | 19720327 <-- |
| CS 161941 | B2 | 19750610 | CS 1972-89 | 19720327 <-- |
| CS 161942 | B2 | 19750610 | CS 1972-90 | 19720327 <-- |
| CS 161939 | B2 | 19750610 | CS 1972-2044 | 19720327 <-- |
| GB 1347203 | A | 19740220 | GB 1972-14446 | 19720328 <-- |
| BE 781791 | A1 | 19721009 | BE 1972-116042 | 19720407 <-- |
| DD 97419 | A5 | 19730514 | DD 1972-162151 | 19720407 <-- |
| AT 321476 | B | 19750410 | AT 1972-3043 | 19720407 <-- |
| AT 7401361 | A | 19750715 | AT 1972-136174 | 19720407 <-- |
| AT 7401362 | A | 19750715 | AT 1972-136274 | 19720407 <-- |
| AT 7401363 | A | 19750715 | AT 1972-136374 | 19720407 <-- |
| CA 973874 | A1 | 19750902 | CA 1972-139185 | 19720407 <-- |
| DK 131867 | B | 19750915 | DK 1972-1726 | 19720407 <-- |
| PL 83556 | B1 | 19751231 | PL 1972-154624 | 19720408 <-- |
| US 3838147 | A | 19740924 | US 1972-242741 | 19720410 <-- |
| HU 168819 | B | 19760728 | HU 1972-ME1485 | 19720410 <-- |
| AT 329194 | B | 19760426 | AT 1974-1361 | 19740219 <-- |
| AT 329195 | B | 19760426 | AT 1974-1362 | 19740219 <-- |
| AT 329196 | B | 19760426 | AT 1974-1363 | 19740219 <-- |

PRIORITY APPLN. INFO.: DE 1971-2117577 A 19710410
DE 1972-2205002 A 19720203
AT 1972-3043 A 19720407

GI For diagram(s), see printed CA Issue.
AB About 30 title compds. (I; R = e.g. Ph, 2-furyl, 2-thienyl, or substituted phenyl; n = 1-3, m = 0 or 1; R1 = e.g. H, Cl, Me2N) were prepared by amination of the corresponding 6-chloro- or 6-methylthiopurine derivs. in the presence of Et3N in a solvent, e.g. Me2CHOH, at room temperature or at reflux or in the melt without solvent. I (R = Ph, n = 2, m = 0, R1 = H) and coronary dilating activity at 0.1-0.5 mg/kg i.v. administered and 80-100% analgesic activity for 30-180 min at 0.1-1.0 mg/kg i.v. in narcotized dogs. I were also useful as circulatory, lipolysis inhibiting, and anticholesteremic drugs.
OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

L3 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1973:136628 CAPLUS

DOCUMENT NUMBER: 78:136628
ORIGINAL REFERENCE NO.: 78:21961a,21964a
TITLE: Heterocyclic-substituted adenosines
INVENTOR(S): Pohlke, Rolf; Mehrhof, Werner; Nowak, Herbert; Simane, Zdenek; Becker, Karl Heinz; Schliep, Hans Jochen
PATENT ASSIGNEE(S): Merck Patent G.m.b.H.
SOURCE: Ger. Offen., 40 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 2139107 | A1 | 19730215 | DE 1971-2139107 | 19710804 <-- |

PRIORITY APPLN. INFO.: DE 1971-2139107 19710804

AB Sixteen title compds. (I; R = H, NH2; R1 = substituted 2-pyridylmethyl, 3-quinolyl, 2-benzodioxanylmethyl, 3-benzothienylmethyl, 2-benzoylfurylmethyl, 2-indolylmethyl, 1-isoquinolylmethyl, 1-piperazinyl, ect.) were prepared by treatment of 6-chloro-9-β-D-ribofuranosylpurine (II) or the 2-amino derivative with the corresponding heterocyclic amine. I were also prepared by reacting the heterocyclic amine with acetylated II, followed by deacetylation with NaOMe.

OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)

L3 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1973:30156 CAPLUS
DOCUMENT NUMBER: 78:30156
ORIGINAL REFERENCE NO.: 78:4771a,4774a
TITLE: Adenosine derivatives
INVENTOR(S): Pohlke, Rolf; Jonas, Rochus; Mehrhof, Werner; Schliep, Hans Jochen; Becker, Karl Heinz; Nowak, Herbert; Simane, Zdenek
PATENT ASSIGNEE(S): Merck Patent G.m.b.H.
SOURCE: Ger. Offen., 36 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 2117577 | A | 19721026 | DE 1971-2117577 | 19710410 <-- |
| ZA 7201889 | A | 19730328 | ZA 1972-1889 | 19720320 <-- |
| NL 7203984 | A | 19721012 | NL 1972-3984 | 19720324 <-- |
| IL 39080 | A | 19750625 | IL 1972-39080 | 19720326 <-- |
| CS 161940 | B2 | 19750610 | CS 1972-88 | 19720327 <-- |
| CS 161941 | B2 | 19750610 | CS 1972-89 | 19720327 <-- |
| CS 161942 | B2 | 19750610 | CS 1972-90 | 19720327 <-- |
| CS 161939 | B2 | 19750610 | CS 1972-2044 | 19720327 <-- |
| GB 1347203 | A | 19740220 | GB 1972-14446 | 19720328 <-- |
| BE 781791 | A1 | 19721009 | BE 1972-116042 | 19720407 <-- |
| DD 97419 | A5 | 19730514 | DD 1972-162151 | 19720407 <-- |
| AT 321476 | B | 19750410 | AT 1972-3043 | 19720407 <-- |
| AT 7401361 | A | 19750715 | AT 1972-136174 | 19720407 <-- |
| AT 7401362 | A | 19750715 | AT 1972-136274 | 19720407 <-- |

| | | | | | | |
|---|---|---|---|---|---|---|
| AT 7401363 | A | 19750715 | AT 1972-136374 | | 19720407 | <-- |
| CA 973874 | A1 | 19750902 | CA 1972-139185 | | 19720407 | <-- |
| DK 131867 | B | 19750915 | DK 1972-1726 | | 19720407 | <-- |
| FR 2132811 | A5 | 19721124 | FR 1972-12452 | | 19720410 | <-- |
| FR 2132811 | B1 | 19750425 | | | | |
| BR 7202095 | D0 | 19730717 | BR 1972-2095 | | 19720410 | <-- |
| US 3838147 | A | 19740924 | US 1972-242741 | | 19720410 | <-- |
| HU 168819 | B | 19760728 | HU 1972-ME1485 | | 19720410 | <-- |
| AT 329194 | B | 19760426 | AT 1974-1361 | | 19740219 | <-- |
| AT 329195 | B | 19760426 | AT 1974-1362 | | 19740219 | <-- |
| AT 329196 | B | 19760426 | AT 1974-1363 | | 19740219 | <-- |

PRIORITY APPLN. INFO.: DE 1971-2117577 A 19710410
DE 1972-2205002 A 19720203
AT 1972-3043 A 19720407

GI For diagram(s), see printed CA Issue.

AB Ten N6-norcamphanyladenosine derivs. (I; R = H, Cl, NH2, NHNH2, SCH2Ph; R1 = H, CH2Ph, Ac; Z = CH2, -) were prepared from 6-chloro-9-(β-D-ribofuranosyl)purine (II) and the correspondingly substituted 2-norcamphanylamine. 3-Phenyl-2-norcamphanylamine reacted with II at 120° to give I (R = R1 = H, Z = -). Condensation was also obtained in alc. containing Et3N at room temperature Adenosine reacted with 2-(chloromethyl)-3-phenylnorcamphane in DMF at 80° to give I (R = R1 = H, Z = CH2). N6-(3-Phenylbicyclo[2.2.1]hept-5-en-2-yl)- and N6-(3-phenylbicyclo[2.2.2]oct-2-yl)-adenosine were also prepared I were useful as hypertensive agents.

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

L3 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1972:565020 CAPLUS
DOCUMENT NUMBER: 77:165020
ORIGINAL REFERENCE NO.: 77:27111a,27114a
TITLE: Polynucleotides. XIV. Synthesis and properties of polynucleotides containing 2,6-bis(methylthio)purine ribonucleotides
AUTHOR(S): Ikehara, Morio; Hattori, Masao
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Toyonaka, Japan
SOURCE: Biochimica et Biophysica Acta, Nucleic Acids and Protein Synthesis (***1972***), 281(1), 11-17
CODEN: BBNPAS; ISSN: 0005-2787
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Homo- and copolynucleotides containing 2,6-bis(methylthio)purine 9-ribonucleoside (ms22,6Pu) were synthesized by polynucleotide phosphorylase. Poly(ms22,6Pu) has a well stacked structure in the neutral solution as studied by CD spectra. The polymer is digestible with ribonuclease M and shows hyperchromicities as high as 42.2 and 83 at 260 and 300 nm, resp. A copolymer, poly(ms22,6PuG), formed a double helical complex with poly(C) without forming loops.

L3 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1969:97105 CAPLUS
DOCUMENT NUMBER: 70:97105
ORIGINAL REFERENCE NO.: 70:18161a,18164a
TITLE: Synthesis of 6-mercaptopurine 2'-deoxyribonucleoside and related compounds and their biological activities
AUTHOR(S): Honjo, Mikio; Furukawa, Yoshiyasu; Yoshioka, Yoshio; Imada, Akira; Fujii, Shoichiro; Ootsu, Koichiro;

Kimura, Takanobu; Komeda, Tomohiko; Matsumoto, Takao
CORPORATE SOURCE: Res. Develop. Div., Takeda Chem. Ind., Ltd., Osaka, Japan
SOURCE: Ann. Rep. Takeda Res. Lab. (**1968**), 27, 1-19
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB Enzymic synthesis of 9-(2-deoxy-β-D-erythro-pentofuranosyl)-6-mercaptopurine (I), m. 180-1° (60% MeOH), [α]2D2 -13.6° (c 1.6, N NaOH), from 6-mercaptopurine (II) and thymidine followed by methylation afforded 6-methylthiopurine 2'-deoxy-D-erythro-pentonucleoside, m. 155-6° (MeOH). Similarly, 2,6-dimethylthiopurine D-ribonucleoside, m. 115-20° (EtOH), [α]2D3 -23.6° (c 0.5, EtOH), was prepared from 2,6-dimethylthiopurine and uridine. 6-Mercaptopurine 2'-deoxy-D-erythro-pentonucleoside 3',5'-cyclic phosphate (III), m. 148-50° (H2O), [α]22D -72° (c 1.1, 0.1N NaOH), was chemical synthesized from 2'-deoxyadenosine 5'-phosphate. Methylation of III gave 6-methylthiopurine 2'-deoxyribonucleoside 3',5'-cyclic phosphate, [α]2D7 -49.2° (c 0.5, H2O). 6-Mercaptopurine 2'-deoxyribonucleoside 5'-phosphate was prepared by enzymic hydrolysis of III. Antitumor activities of I and II were assessed for several kinds of animal tumor. The antitumor activity of I against adenocarcinoma 755 was about the same as that of II at equimolar doses.

L3 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1965:411280 CAPLUS
DOCUMENT NUMBER: 63:11280
ORIGINAL REFERENCE NO.: 63:2030b-d
TITLE: Interaction between synthetic adenosine triphosphate analogs and actomyosin systems. III
AUTHOR(S): Ikehara, Morio; Ohtsuka, Eiko; Uno, Hitoshi; Imamura, Kiichi; Tonomura, Yuji
CORPORATE SOURCE: Hokkaido Univ., Sapporo, Japan
SOURCE: Biochimica et Biophysica Acta, General Subjects (**1965**), 100(2), 471-8
CODEN: BBGSB3; ISSN: 0304-4165
DOCUMENT TYPE: Journal
LANGUAGE: English
AB cf. CA 60, 7060a. The following compds. were synthesized as analogs of ATP: 6-morpholino-9-(2',3'-O-isopropylidene)-β D-ribofuranosylpyrine 5'-triphosphate (I) and 2,6dimethylmercapto-9-β-ribofuranosylpurine 5'-triphosphate (II). The interactions of these analogs with actomyosin systems were investigated, together with those of 3'-deoxythymidine 5'-triphosphate (III), thymidine 5'-triphosphate (IV), and 2',3'-O-isopropylideneadenosine 5'-triphosphate (V). The degrees of decrease in light-scattering of myosin B on addition of these analogs were similar to that induced by ATP, except in the case of III. The rates of hydrolysis of analogs by myosin B in 0.6M KCl and 7 mM Ca2+ were in the decreasing order of ATP > V ≈ IV > II > III ≈ II, while the order of hydrolysis in 0.075M KCl and 2mMMg2+ was IV > ATP > V > III > II > II. IV and V, as well as ATP, induced contraction of myofibrils, while I, II, and III did not. It was concluded that H bondings at the N-6 or O of the base and the 0-3 of ribose with myosin are necessary for the rapid hydrolysis of an ATP analog and for contraction of myofibrils by the analog.
OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

L3 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1963:409279 CAPLUS
DOCUMENT NUMBER: 59:9279
ORIGINAL REFERENCE NO.: 59:1742c-g
TITLE: Potential antimetabolites. IV. Synthesis of 2,6-bis(alkylthio)purine ribosides and their selective substitution by nucleophilic reagents
AUTHOR(S): Ikehara, Morio; Ueda, Tohru; Horikawa, Sumiko; Yamazaki, Akihiro
CORPORATE SOURCE: Hokkaido Univ., Sapporo, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (***1962***), 10, 665-9
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB 2-Mercaptohypoxanthine was thiolated with P2S5 in C5H5N according to the modified method of Fox, et al. (CA 52, 13736i) to yield 85% crude 2,6-dimercaptopurine, which was alkylated by stirring 2 hrs. with PhCH2Cl in 2N NaOH to 73.4% 1,6-bis(benzylthio)purine (I). The mother liquor from I gave a tribenzyl derivative (II), probably the 9-PhCH2 deriv, of I, m. 143-4°. Mixing equimolar amts. of I, 10% NaOH, and HgCl2 in EtOH gave the HgCl salt of I, and this was suspended in xylene, refluxed 3 hrs. with 2,3,5-O-benzoyl-D-ribofuranosyl chloride in C6H6, evaporated below 40° to a red sirup, which was purified by extraction with CHCl3 and Al2O3 chromatography to yield 16% IIa (R = PhCH2) (III), m. 139-40°, [α]15D -43.4° (c 0.465, dioxane). III was debenzoylated by keeping 2 days at room temperature with cyclohexylamine in MeOH, then refluxing the mixture, and evaporating to give a quant. yield of 2,6-bis(benzylthio)-9-β-D-ribofuranosylpurine (IV), m. 133-5°, [α]15D -16.1° (c 0.36, MeOH). By procedures similar to those used with I and its derivs., 2,6-bis(methylthio)purine was converted to its HgCl salt, m. above 200° (decomposition), in 95% yield, and this to 37% IIa (R = Me) (V), m. 70-80°, [α]19D -25.0°. III and V sep. heated in a sealed tube at 100° with 33% Me2NH 3 hrs. and 12 hrs., resp., yielded 64% 2-PhCH2S derivative (VI) and 46% 2-MeS derivative (VII) of 6-dimethylamino-9-β-D-ribofuranosylpurine (VIII), m. 185-6° and 171-2°, resp. VI [[α]20D -44.5° (c 0.805, MeOH)] was also obtained from IV in 84% yield by similar treatment. Desulfurization of VI and VII was carried out by refluxing 2.5 hrs. with Raney Ni in EtOH to yield 42.5 and 57% VIII, resp., m. 180-1°. V (1.3 g.) heated 4.5 hrs. in a sealed tube at 100° with MeNH2 (in place of Me2NH) yielded 0.3 g. 6-methylamino-2-methylthio-9-β-D-ribofuranosylpurine (IX); picrate m. 158-60° (rapid heating), or 223° (decomposition) (gentle heating). IX refluxed 5 hrs. with Raney Ni in EtOH also yielded VIII, 50 mg. from 200 mg. IX. Ultraviolet absorption maximum and min. were reported for I-IX in support of their structures.

L3 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1959:11835 CAPLUS
DOCUMENT NUMBER: 53:11835
ORIGINAL REFERENCE NO.: 53:2236a-i,2237a
TITLE: Synthesis of potential anticancer agents. XIV. Ribosides of 2,6-disubstituted purines
AUTHOR(S): Schaeffer, Howard J.; Thomas, H. Jeanette
CORPORATE SOURCE: Southern Research Inst., Birmingham, AL
SOURCE: Journal of the American Chemical Society (***1958***), 80, 3738-42
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 53:11835

AB cf. C.A. 52, 10104e. 2,6-Dichloropurine (1.60 g.), 2.40 g. Celite, 1.14 g. $HgCl_2$, and 210 cc. 50% aqueous EtOH treated slowly with stirring with 3.04 cc. 10% aqueous NaOH, cooled overnight, and filtered, and the residue washed and dried 8 hrs. at 61°/3 mm. over $P_2O_5$ yielded 4.80 g. mixture of 2.40 g. Celite and 2.40 g. bis(2,6-dichloropurinyl)mercury (I). 2,3,5-Tri-O-benzoyl-D-ribofuranosyl chloride from 7.67 g. 1-O-acetyl-2,3,5-tri-O-benzoyl-β-ribose in 50 cc. xylene added to 4.38 g. I and 4.60 g. Celite in 400 cc. dry xylene, refluxed 2 hrs. with stirring and filtered, the filter cake washed with hot $CHCl_3$, the xylene filtrate evaporated, the residue dissolved in hot $CHCl_3$, and the combined $CHCl_3$ solns. washed with 30% aqueous KI and $H_2O$, dried, treated with C, and concentrated yielded 9.93 g. 2,6-dichloro-9-(2,3,5-tri-O-benzoyl)-β-D-ribofuranosylpurine (II), tan glass. Crude II (2.11 g.) in 100 cc. absolute MeOH refluxed 1 hr., neutralized with AcOH, and evaporated in vacuo, the residue dissolved in 30 cc. $H_2O$ and extracted with $CHCl_3$, the aqueous solution evaporated to leave 800 mg. gel, and a 200-mg. portion subjected to a partition chromatography on Celite with $H_2O$-saturated BuOH yielded 140 mg. 2-chloro-6-methoxy-9-β-D-ribofuranosylpurine (III), m. 140° (iso-PrOH-EtOAc), $[\alpha]_D^{26}$ -30.4 ± 2.3° (c 0.612, MeOH). III (308 mg.) in 50 cc. 50% aqueous MeOH hydrogenated under ambient conditions 39 min. over 100 mg. 5% Pd-C and 40 mg. MgO gave 203 mg. 6-methoxy-9-β-D-ribofuranosylpurine, m. 140° (MeOH-EtOAc). III (176 mg.) in 15 cc. MeOH (saturated with $NH_3$ at 0°) heated 16 hrs. at 83° in a steel bomb, filtered, and evaporated in vacuo, the residue dissolved in $H_2O$, the solution treated with 10 cc. 14% aqueous picric acid, the precipitate filtered off and dissolved in $H_2O$, the aqueous solution stirred with 0.3 g. Dowex 1 ($CO_3$) and filtered, and the filtrate evaporated yielded 61 mg. 6-amino-2-chloro-9-β-D-ribofuranosylpurine (IV), m. 145-6° (decomposition). III (500 mg.) in 75 cc. MeOH treated with 3.16 cc. N NaSMe in MeOH, refluxed 2 hrs., cooled, neutralized with N HCl, and evaporated in vacuo, and the residue dissolved in hot $H_2O$ and cooled yielded 203 mg. amorphous 2-MeS analog of III, m. 160-1° with softening at 116°, $[\alpha]_D^{26}$ -16.9 ± 2.1° (c 0.649, MeOH); 2nd crop, 140 mg. III (500 mg.) in 75 cc. MeOH refluxed 4 hrs. with 3.16 cc. N NaOMe, neutralized with N HCl, and evaporated in vacuo, and the residue recrystd. from $H_2O$ and dried 24 hrs. at 110°/0.08 mm. over $P_2O_5$ gave 155 mg. 2,6-dimethoxy-9-β-D-ribofuranosylpurine, m. 163° with softening at 120°, $[\alpha]_D^{32}$ -33.6 ± 2.2° (c 0.648, MeOH). Crude II (6.00 g.) and 420 cc. MeOH (saturated at 0° with $NH_3$) stirred to solution, kept overnight, and evaporated in vacuo, the residue dissolved in 40 cc. $H_2O$, washed with $CHCl_3$, treated with 25 cc. 11% aqueous picric acid, and filtered, the residue dissolved in $H_2O$, the solution stirred with 9 g. Dowex 1 ($CO_3$) resin and filtered, and the filtrate concentrated to 20 cc. gave 670 mg. IV, m. 142° (decomposition). IV (302 mg.) in 50 cc. MeOH refluxed 16 hrs. with 2 cc. N NaOMe, cooled, neutralized with N HCl, and evaporated in vacuo, and the residue recrystd. from $H_2O$ yielded 104 mg. 2-MeO analog of IV, m. 190-2° (decomposition), $[\alpha]_D^{26}$ -43.3 ± 2.3° (c 0.610, MeOH). IV (300 mg.) in 50 cc. PrOH treated with 2.0 cc. N NaSMe in PrOH, refluxed 2.5 hrs., neutralized with N HCl, and filtered, and the filtrate evaporated in vacuo yielded 119 mg. 2-MeS analog of IV, m. 153° resolidified 185-90° and remelted 220° (decomposition). IV (302 mg.) in 10 cc. 25% aqueous $Me_2NH$ diluted with 35 cc. MeOH, heated 16 hrs. in a bomb at

100°, and evaporated in vacuo, and the residue crystallized from 40 cc. H2O yielded 221 mg. 2-Me2N analog of IV, m. 213° (decomposition). IV (302 mg.) in 10 cc. 40% aqueous MeNH2 diluted with 35 cc. MeOH and heated 4 hrs. in a bomb at 100°, the solution evaporated to dryness, and the residue crystal. from MeOH-EtOAc yielded 116 mg. 2-MeNH analog of IV, m. 198° (decomposition), [α]26D -42.8 ± 3.3° (c 0.416, MeOH). IV (602 mg.) added in portions to 30 cc. N2H4, kept 16 hrs. at room temperature under N, and evaporated in vacuo at 30°, and the residue evaporated 3 times with 15-cc. portions iso-PrOH and recrystd. yielded 225 mg. 2-H2NNH analog (V) of IV, m. 143° resolidified at 150-5° and remelted at 200° with decomposition (2nd crop, 51 mg.), [α]26D -33.0 ± 1.8° (c 0.763, H2O). V (297 mg.) in 7 cc. 5% aqueous AcOH treated with cooling with 83 mg. NaNO2 in 17 cc. H2O, cooled 1 hr., and filtered, and the residue (218 mg.) recrystd. from H2O and dried 48 hrs. at 100°/0.07 mm. over P2O5 yielded 142 mg. 2-N2 analog of IV, m. 159-60° (decomposition), [α]26D -27.6 ± 5.8° (c 0.232, MeOH).

OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)

=> d his

(FILE 'HOME' ENTERED AT 13:32:42 ON 12 NOV 2010)

FILE 'REGISTRY' ENTERED AT 13:32:52 ON 12 NOV 2010
E XANTHOSINE, 2,6-/CN
L1 6 S E4,E5, E6,E7,E8,E9

FILE 'CAPLUS' ENTERED AT 13:34:15 ON 12 NOV 2010
L2 18 S L1
L3 17 S L2 AND PY<= 2003

=> logoff hold

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 55.51 | 89.71 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | -14.45 | -14.45 |

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 13:34:53 ON 12 NOV 2010